Diannan Lu

List of Publications by Year in Descending Order

96 papers	1,897 citations	26 h-index	40 g-index
105 ext. papers	2,198 ext. citations	5.4 avg, IF	4.92 L-index

#	Paper	IF	Citations
96	Diffusion and Entropy of Supercooled Water in Nanoslit. *Chemical Engineering Journal*, **2022**, 446, 136672	14.7	
95	Theoretical insights on the hydration of quinones as catholytes in aqueous redox flow batteries. *Chinese Journal of Chemical Engineering*, **2021**, 37, 72-72	3.2	0
94	Ecological Response in the Integrated Process of Biostimulation and Bioaugmentation of Diesel-Contaminated Soil. *Applied Sciences (Switzerland)*, **2021**, 11, 6305	2.6	
93	The synergistic mechanisms of apo-ferritin structural transitions and Au(iii) ion transportation: molecular dynamics simulations with the Markov state model. *Physical Chemistry Chemical Physics*, **2021**, 23, 17158-17165	3.6	0
92	An improved batch fluidized drying experimental design based on digital sensors and a minicomputer. *Engineering Reports*, **2021**, 3, e12366	1.2	1
91	A distal regulatory strategy of enzymes: from local to global conformational dynamics. *Physical Chemistry Chemical Physics*, **2021**, 23, 22451-22465	3.6	0
90	Global and Kinetic Profiles of Substrate Diffusion in Lipase B: Molecular Dynamics with the Markov-State Model. *ACS Omega*, **2020**, 5, 9806-9812	3.9	4
89	Design of Multinuclear Gold Binding Site at the Two-fold Symmetric Interface of the Ferritin Cage. *Chemistry Letters*, **2020**, 49, 840-844	1.7	1
88	A Multiscale Procedure for Predicting the Hydration Free Energies of Polycyclic Aromatic Hydrocarbons. *Journal of Chemical & Engineering Data*, **2020**, 65, 2206-2211	2.8	3
87	Laterally Heterogeneous 2D Layered Materials as an Artificial Light-Harvesting Proton Pump. *Advanced Functional Materials*, **2020**, 30, 2001549	15.6	6
86	A hybrid theoretical method for predicting electrokinetic energy conversion in nanochannels. *Physical Chemistry Chemical Physics*, **2020**, 22, 9110-9116	3.6	0
85	Electric-Field-Induced Ionic Sieving at Planar Graphene Oxide Heterojunctions for Miniaturized Water Desalination. *Advanced Materials*, **2020**, 32, e1903954	24	34
84	Increased stability and intracellular antioxidant activity of chlorogenic acid depend on its molecular interaction with wheat gluten hydrolysate. *Food Chemistry*, **2020**, 325, 126873	8.5	8
83	Photoinduced Directional Proton Transport through Printed Asymmetric Graphene Oxide Superstructures: A New Driving Mechanism under Full-Area Light Illumination. *Advanced Functional Materials*, **2020**, 30, 1907549	15.6	13
82	Light-Powered Directional Nanofluidic Ion Transport in Kirigami-Made Asymmetric Photonic-Ionic Devices. *Small*, **2020**, 16, e1905557	11	8
81	Computational screening and design of nanoporous membranes for efficient carbon isotope separation. *Green Energy and Environment*, **2020**, 5, 364-373	5.7	2
80	Recent progress in enzymatic functionalization of carbon-hydrogen bonds for the green synthesis of chemicals. *Chinese Journal of Chemical Engineering*, **2020**, 28, 2499-2506	3.2	0

79	Single-molecule level dynamic observation of disassembly of the apo-ferritin cage in solution. *Physical Chemistry Chemical Physics*, **2020**, 22, 18562-18572	3.6	6
78	Graphene oxide enabled long-term enzymatic transesterification in an anhydrous gas flux. *Nature Communications*, **2019**, 10, 2684	17.4	22
77	Recent progresses in the accumulation of metal ions into the apo-ferritin cage: Experimental and theoretical perspectives. *Polyhedron*, **2019**, 172, 104-111	2.7	8
76	Photo-induced ultrafast active ion transport through graphene oxide membranes. *Nature Communications*, **2019**, 10, 1171	17.4	82
75	Coordination design of cadmium ions at the 4-fold axis channel of the apo-ferritin cage. *Dalton Transactions*, **2019**, 48, 9759-9764	4.3	4
74	Light-Driven Active Proton Transport through Photoacid- and Photobase-Doped Janus Graphene Oxide Membranes. *Advanced Materials*, **2019**, 31, e1903029	24	42
73	How pressure affects confine water inside different nanoslits.. *RSC Advances*, **2019**, 9, 19086-19094	3.7	2
72	Highly Efficient Ionic Photocurrent Generation through WS -Based 2D Nanofluidic Channels. *Small*, **2019**, 15, e1905355	11	23
71	How Serratia marcescens HB-4 absorbs cadmium and its implication on phytoremediation. *Ecotoxicology and Environmental Safety*, **2019**, 185, 109723	7	7
70	Intensification of chemical separation engineering by nanostructured channels and nanofluidics: From theories to applications. *Chinese Journal of Chemical Engineering*, **2019**, 27, 1439-1448	3.2	5
69	Molecular dynamics simulations reveal how graphene oxide stabilizes and activates lipase in an anhydrous gas. *Physical Chemistry Chemical Physics*, **2019**, 21, 25425-25430	3.6	5
68	Isolation and characterization of a quinclorac-degrading Actinobacteria Streptomyces sp. strain AH-B and its implication on microecology in contaminated soil. *Chemosphere*, **2018**, 199, 210-217	8.4	14
67	Markov-state model for CO binding with carbonic anhydrase under confinement. *Journal of Chemical Physics*, **2018**, 148, 035101	3.9	3
66	Valorization of food waste into biofertiliser and its field application. *Journal of Cleaner Production*, **2018**, 187, 273-284	10.3	66
65	A molecular theory for predicting the thermodynamic efficiency of electrokinetic energy conversion in slit nanochannels. *Journal of Chemical Physics*, **2018**, 148, 084701	3.9	7
64	The Mechanism for siRNA Transmembrane Assisted by PMAL. *Molecules*, **2018**, 23,	4.8	1
63	Detachment of HCO_3^- from the Active Site of Carbonic Anhydrase: Molecular Dynamics Simulation and Machine Learning. *Journal of Physical Chemistry C*, **2018**, 122, 20539-20549	3.8	3
62	Magnetic Multienzyme Nanoparticles Catalyzed Degradation of Aqueous Tributyltin. *Catalysis Letters*, **2018**, 148, 3732-3740	2.8	0

61	Bioadsorption and biostabilization of cadmium by Enterobacter cloacae TU. *Chemosphere*, **2017**, 173, 622-629	8.4	37
60	Biodegradation of chlorothalonil by Enterobacter cloacae TUAH-1. *International Biodeterioration and Biodegradation*, **2017**, 121, 122-130	4.8	8
59	A theoretical study on the morphological phase diagram of supported lipid bilayers. *Physical Chemistry Chemical Physics*, **2017**, 19, 16897-16903	3.6	1
58	Kinetics of CO diffusion in human carbonic anhydrase: a study using molecular dynamics simulations and the Markov-state model. *Physical Chemistry Chemical Physics*, **2017**, 19, 11690-11697	3.6	7
57	Preparation of uniform magnetic iron oxide nanoparticles by co-precipitation in a helical module microchannel reactor. *Journal of Environmental Chemical Engineering*, **2017**, 5, 303-309	6.8	22
56	The mechanism for the complexation and dissociation between siRNA and PMAL: a molecular dynamics simulation study based on a coarse-grained model. *Molecular Simulation*, **2017**, 43, 1385-1393	2	5
55	Predicting hydration free energies of amphetamine-type stimulants with a customized molecular model. *Journal of Physics Condensed Matter*, **2016**, 28, 344001	1.8	4
54	Spreading of a Unilamellar Liposome on Charged Substrates: A Coarse-Grained Molecular Simulation. *Langmuir*, **2016**, 32, 3785-93	4	11
53	A multi-scale molecular dynamics simulation of PMAL facilitated delivery of siRNA. *RSC Advances*, **2015**, 5, 68227-68233	3.7	11
52	Molecular dynamics for the charging behavior of nanostructured electric double layer capacitors containing room temperature ionic liquids. *Nano Research*, **2015**, 8, 931-940	10	15
51	How ABA block polymers activate cytochrome c in toluene: molecular dynamics simulation and experimental observation. *Physical Chemistry Chemical Physics*, **2015**, 17, 10708-14	3.6	5
50	A molecular theory for optimal blue energy extraction by electrical double layer expansion. *Physical Chemistry Chemical Physics*, **2015**, 17, 23970-6	3.6	14
49	Kinetic and multidimensional profiling of accelerated degradation of oil sludge by biostimulation. *Environmental Sciences: Processes and Impacts*, **2015**, 17, 763-74	4.3	15
48	Italicized carbon nanotube facilitating water transport: a molecular dynamics simulation. *Science Bulletin*, **2015**, 60, 1580-1586	10.6	12
47	Uniform mPEG-b-PMETAC enables pH-responsive delivery of insulin. *Journal of Applied Polymer Science*, **2015**, 132, n/a-n/a	2.9	4
46	Enzymatic Synthesis of High-Molecular-Weight Poly(butylene succinate) and its Copolymers. *Macromolecular Chemistry and Physics*, **2015**, 216, 636-640	2.6	26
45	Surface tension effects on the phase transition of a DPPC bilayer with and without protein: a molecular dynamics simulation. *Physical Chemistry Chemical Physics*, **2014**, 16, 8434-40	3.6	8
44	Ecological and enzymatic responses to petroleum contamination. *Environmental Sciences: Processes and Impacts*, **2014**, 16, 1501-9	4.3	34

43	Electrokinetic desalination using honeycomb carbon nanotubes (HC-CNTs): a conceptual study by molecular simulation. *Physical Chemistry Chemical Physics*, **2014**, 16, 18941-8	3.6	6
42	Multiscale simulation of surfactant–aquaporin complex formation and water permeability. *RSC Advances*, **2014**, 4, 37592-37599	3.7	4
41	Molecular Theory for Electrokinetic Transport in pH-Regulated Nanochannels. *Journal of Physical Chemistry Letters*, **2014**, 5, 3015-20	6.4	23
40	Design and synthesis of lipase nanogel with interpenetrating polymer networks for enhanced catalysis: Molecular simulation and experimental validation. *Journal of Molecular Catalysis B: Enzymatic*, **2013**, 88, 60-68		9
39	Accelerating water transport through a charged SWCNT: a molecular dynamics simulation. *Physical Chemistry Chemical Physics*, **2013**, 15, 14447-57	3.6	23
38	Reversible encapsulation of lysozyme within mPEG-b-PMAA: experimental observation and molecular dynamics simulation. *Soft Matter*, **2013**, 9, 8723	3.6	14
37	Substrate imprinted lipase nanogel for one-step synthesis of chloramphenicol palmitate. *Green Chemistry*, **2013**, 15, 1155	10	38
36	Temperature-responsive enzyme-polymer nanoconjugates with enhanced catalytic activities in organic media. *Chemical Communications*, **2013**, 49, 6090-2	5.8	56
35	Pathways for degrading TNT by Thu-Z: a Pantoea sp. strain. *Applied Biochemistry and Biotechnology*, **2012**, 168, 1976-88	3.2	8
34	Magnetic enzyme nanogel (MENG): a universal synthetic route for biocatalysts. *Chemical Communications*, **2012**, 48, 3315-7	5.8	41
33	Nanobiocatalysis in Organic Media: Opportunities for Enzymes in Nanostructures. *Topics in Catalysis* , **2012**, 55, 1070-1080	2.3	33
32	Activation and stabilization of a lipase nanogel using GMA for acryloylation. *Soft Matter*, **2012**, 8, 2036	3.6	9
31	How hydrophobicity and the glycosylation site of glycans affect protein folding and stability: a molecular dynamics simulation. *Journal of Physical Chemistry B*, **2012**, 116, 390-400	3.4	39
30	Strengthening the stability of a tunnel-shaped homotetramer protein with nanogels. *Journal of Physical Chemistry B*, **2011**, 115, 8875-82	3.4	7
29	How PEGylation enhances the stability and potency of insulin: a molecular dynamics simulation. *Biochemistry*, **2011**, 50, 2585-93	3.2	98
28	Refolding of inclusion body proteins from E. coli. *Methods of Biochemical Analysis*, **2011**, 54, 319-38		10
27	Restoration of taxonomic and functional genes after bioaugmentation of petroleum contaminated soil. *Journal of Environmental Monitoring*, **2011**, 13, 2904-13		4
26	Uniform polymer-protein conjugate by aqueous AGET ATRP using protein as a macroinitiator. *Acta Biomaterialia*, **2011**, 7, 2131-8	10.8	31

25	Enriched microbial community in bioaugmentation of petroleum-contaminated soil in the presence of wheat straw. *Applied Biochemistry and Biotechnology*, **2011**, 164, 1071-82	3.2	14
24	A lipase-responsive vehicle using amphipathic polymer synthesized with the lipase as catalyst. *Macromolecular Rapid Communications*, **2011**, 32, 546-50	4.8	32
23	Studies of protein folding pathways. *Annual Reports on the Progress of Chemistry Section C*, **2010**, 106, 259		1
22	Dynamic control of protein conformation transition in chromatographic separation based on hydrophobic interactions: molecular dynamics simulation. *Journal of Chromatography A*, **2009**, 1216, 2483-90	4.5	14
21	Recent advances in nanostructured biocatalysts. *Biochemical Engineering Journal*, **2009**, 44, 53-59	4.2	137
20	Lipase nanogel catalyzed transesterification in anhydrous dimethyl sulfoxide. *Biomacromolecules*, **2009**, 10, 1612-8	6.9	95
19	Strengthening intersubunit hydrogen bonds for enhanced stability of recombinant urate oxidase from Aspergillus flavus: molecular simulations and experimental validation. *Physical Chemistry Chemical Physics*, **2009**, 11, 333-40	3.6	10
18	Preparation and Antibacterial Function of Quaternary Ammonium Salts Grafted Cellulose Fiber Initiated by Fe2 +-H2O2 Redox. *Journal of Macromolecular Science - Pure and Applied Chemistry*, **2009**, 46, 560-565	2.2	4
17	Oscillatory molecular driving force for protein folding at high concentration: a molecular simulation. *Journal of Physical Chemistry B*, **2008**, 112, 2686-93	3.4	12
16	Molecular fundamentals of enzyme nanogels. *Journal of Physical Chemistry B*, **2008**, 112, 14319-24	3.4	73
15	Dynamic redox environment-intensified disulfide bond shuffling for protein refolding in vitro: molecular simulation and experimental validation. *Journal of Physical Chemistry B*, **2008**, 112, 15127-33	3.4	23
14	How native proteins aggregate in solution: a dynamic Monte Carlo simulation. *Biophysical Chemistry* , **2008**, 133, 71-80	3.5	26
13	Dynamic control of protein folding pathway with a polymer of tunable hydrophobicity. *Journal of Physical Chemistry B*, **2007**, 111, 12303-9	3.4	11
12	Fabrication of single carbonic anhydrase nanogel against denaturation and aggregation at high temperature. *Biomacromolecules*, **2007**, 8, 560-5	6.9	84
11	Protein refolding assisted by periodic mesoporous organosilicas. *Langmuir*, **2007**, 23, 5735-9	4	53
10	Hyperbranched polymer conjugated lipase with enhanced activity and stability. *Biochemical Engineering Journal*, **2007**, 36, 93-99	4.2	42
9	Molecular dynamics for surfactant-assisted protein refolding. *Journal of Chemical Physics*, **2007**, 126, 064906	3.9	10
8	Structural transitions of confined model proteins: molecular dynamics simulation and experimental validation. *Biophysical Journal*, **2006**, 90, 3224-38	2.9	35

7	Dextran-grafted-PNIPAAm as an artificial chaperone for protein refolding. *Biochemical Engineering Journal*, **2006**, 27, 336-343	4.2	37
6	The mechanism of PNIPAAm-assisted refolding of lysozyme denatured by urea. *Biochemical Engineering Journal*, **2005**, 24, 55-64	4.2	33
5	How CTAB assists the refolding of native and recombinant lysozyme. *Biochemical Engineering Journal*, **2005**, 24, 269-277	4.2	36
4	Protein refolding assisted by an artificial chaperone using temperature stimuli responsive polymer as the stripper. *Biochemical Engineering Journal*, **2005**, 25, 141-149	4.2	24
3	Molecular simulation of surfactant-assisted protein refolding. *Journal of Chemical Physics*, **2005**, 122, 134902	3.9	12
2	Molecular simulation of polymer assisted protein refolding. *Journal of Chemical Physics*, **2005**, 123, 134903	3.9	4
1	Ion effects on the extraction of cesium (I) by 1,3-Diisopropoxycalix [4] arenecrown-6(BPC6) and the highly efficient extraction under neutral conditions. *Solvent Extraction and Ion Exchange*,1-16	2.5	1