

# Binquan Luan

## List of Publications by Year in descending order

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85  
papers

4,062  
citations

126858

33  
h-index

123376

61  
g-index

95  
all docs

95  
docs citations

95  
times ranked

5699  
citing authors

#	ARTICLE	IF	CITATIONS
1	Insights into SARS-CoV-2's Mutations for Evading Human Antibodies: Sacrifice and Survival. Journal of Medicinal Chemistry, 2022, 65, 2820-2826.	2.9	49
2	Crystal structures-guided design of fragment-based drugs for inhibiting the main protease of SARS-CoV-2. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1081-1089.	1.5	5
3	Stable Cell Clones Harboring Self-Replicating SARS-CoV-2 RNAs for Drug Screen. Journal of Virology, 2022, 96, jvi0221621.	1.5	14
4	Crown Nanopores in Graphene for CO <sub>2</sub> Capture and Filtration. ACS Nano, 2022, 16, 6274-6281.	7.3	23
5	Understanding interactions between biomolecules and two-dimensional nanomaterials using in silico microscopes. Advanced Drug Delivery Reviews, 2022, 186, 114336.	6.6	22
6	Friction and Plasticity in Contacts Between Amorphous Solids. Tribology Letters, 2021, 69, 1.	1.2	5
7	Enhanced binding of the N501Y-mutated SARS-CoV-2 spike protein to the human ACE2 receptor: insights from molecular dynamics simulations. FEBS Letters, 2021, 595, 1454-1461.	1.3	165
8	Field-Dependent Dehydration and Optimal Ionic Escape Paths for C <sub>2</sub> N Membranes. Journal of Physical Chemistry B, 2021, 125, 7044-7059.	1.2	3
9	Nanopores in Atomically Thin 2D Nanosheets Limit Aqueous Single-Stranded DNA Transport. Physical Review Letters, 2021, 127, 138103.	2.9	13
10	Role of intercalation in the electrical properties of nucleic acids for use in molecular electronics. Nanoscale Horizons, 2021, 6, 651-660.	4.1	10
11	Structure-Function Analysis of Resistance to Bamlanivimab by SARS-CoV-2 Variants Kappa, Delta, and Lambda. Journal of Chemical Information and Modeling, 2021, 61, 5133-5140.	2.5	21
12	Targeting Proteases for Treating COVID-19. Journal of Proteome Research, 2020, 19, 4316-4326.	1.8	68
13	Structure-based lead optimization of herbal medicine rutin for inhibiting SARS-CoV-2's main protease. Physical Chemistry Chemical Physics, 2020, 22, 25335-25343.	1.3	34
14	Electrophoretic Transport of Single-Stranded DNA through a Two Dimensional Nanopore Patterned on an In-Plane Heterostructure. ACS Nano, 2020, 14, 13137-13145.	7.3	19
15	<i>In Silico</i> Antibody Mutagenesis for Optimizing Its Binding to Spike Protein of Severe Acute Respiratory Syndrome Coronavirus 2. Journal of Physical Chemistry Letters, 2020, 11, 9781-9787.	2.1	22
16	<i>In Silico</i> Exploration of the Molecular Mechanism of Clinically Oriented Drugs for Possibly Inhibiting SARS-CoV-2's Main Protease. Journal of Physical Chemistry Letters, 2020, 11, 4413-4420.	2.1	118
17	Potential interference with microtubule assembly by graphene: a tug-of-war. Nanoscale, 2020, 12, 4968-4974.	2.8	7
18	In silico Exploration of Inhibitors for SARS-CoV-2's Papain-Like Protease. Frontiers in Chemistry, 2020, 8, 624163.	1.8	15

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19	Energetically stretching proteins on patterned two dimensional nanosheets. Nano Futures, 2020, 4, 035001.	1.0	3
20	Parameterization of Molybdenum Disulfide Interacting with Water Using the Free Energy Perturbation Method. Journal of Physical Chemistry B, 2019, 123, 7243-7252.	1.2	11
21	Spontaneous ssDNA stretching on graphene and hexagonal boron nitride in plane heterostructures. Nature Communications, 2019, 10, 4610.	5.8	36
22	Combined Computational&#x2013;Experimental Approach to Explore the Molecular Mechanism of SaCas9 with a Broadened DNA Targeting Range. Journal of the American Chemical Society, 2019, 141, 6545-6552.	6.6	31
23	Atomic-Scale Fluidic Diodes Based on Triangular Nanopores in Bilayer Hexagonal Boron Nitride. Nano Letters, 2019, 19, 977-982.	4.5	31
24	Exploring the binding mechanism between human profilin (PFN1) and polyproline-10 through binding mode screening. Journal of Chemical Physics, 2019, 150, 015102.	1.2	4
25	Single Locked Nucleic Acid-Enhanced Nanopore Genetic Discrimination of Pathogenic Serotypes and Cancer Driver Mutations. ACS Nano, 2018, 12, 4194-4205.	7.3	24
26	Spontaneous Transport of Single-Stranded DNA through Graphene&#x2013;MoS <sub>2</sub> Heterostructure Nanopores. ACS Nano, 2018, 12, 3886-3891.	7.3	57
27	Glassy dynamics in mutant huntingtin proteins. Journal of Chemical Physics, 2018, 149, 072333.	1.2	9
28	Single-File Protein Translocations through Graphene&#x2013;MoS <sub>2</sub> Heterostructure Nanopores. Journal of Physical Chemistry Letters, 2018, 9, 3409-3415.	2.1	45
29	Membrane Insertion and Phospholipids Extraction by Graphyne Nanosheets. Journal of Physical Chemistry C, 2017, 121, 2444-2450.	1.5	31
30	High-Curvature Nanostructuring Enhances Probe Display for Biomolecular Detection. Nano Letters, 2017, 17, 1289-1295.	4.5	64
31	Graphene-Induced Pore Formation on Cell Membranes. Scientific Reports, 2017, 7, 42767.	1.6	103
32	PEGylated graphene oxide elicits strong immunological responses despite surface passivation. Nature Communications, 2017, 8, 14537.	5.8	157
33	Molecular Mechanism of Stabilizing the Helical Structure of Huntingtin N17 in a Micellar Environment. Journal of Physical Chemistry B, 2017, 121, 4713-4721.	1.2	11
34	A novel self-activation mechanism of Candida antarctica lipase B. Physical Chemistry Chemical Physics, 2017, 19, 15709-15714.	1.3	18
35	Understanding the graphene quantum dots-ubiquitin interaction by identifying the interaction sites. Carbon, 2017, 121, 285-291.	5.4	17
36	Emerging $\beta$ -Sheet Rich Conformations in Supercompact Huntingtin Exon-1 Mutant Structures. Journal of the American Chemical Society, 2017, 139, 8820-8827.	6.6	43

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37	Humidity-Responsive Single-Nanoparticle-Layer Plasmonic Films. <i>Advanced Materials</i> , 2017, 29, 1606796.	11.1	25
38	Structural perturbations on huntingtin N17 domain during its folding on 2D-nanomaterials. <i>Nanotechnology</i> , 2017, 28, 354001.	1.3	12
39	Detecting Interactions between Nanomaterials and Cell Membranes by Synthetic Nanopores. <i>ACS Nano</i> , 2017, 11, 12615-12623.	7.3	25
40	Bio-nano interactions detected by nanochannel electrophoresis. <i>Electrophoresis</i> , 2016, 37, 2190-2195.	1.3	3
41	Potential disruption of protein-protein interactions by graphene oxide. <i>Journal of Chemical Physics</i> , 2016, 144, 225102.	1.2	24
42	Wettability and friction of water on a MoS2 nanosheet. <i>Applied Physics Letters</i> , 2016, 108, .	1.5	113
43	Mechanism of Divalent-Ion-Induced Charge Inversion of Bacterial Membranes. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2434-2438.	2.1	20
44	Opening Lids: Modulation of Lipase Immobilization by Graphene Oxides. <i>ACS Catalysis</i> , 2016, 6, 4760-4768.	5.5	139
45	Radial dependence of DNA translocation velocity in a solid-state nanopore. <i>Mikrochimica Acta</i> , 2016, 183, 995-1002.	2.5	3
46	Sequential protein unfolding through a carbon nanotube pore. <i>Nanoscale</i> , 2016, 8, 12143-12151.	2.8	17
47	Complete wetting of graphene by biological lipids. <i>Nanoscale</i> , 2016, 8, 5750-5754.	2.8	83
48	Potential Interference of Protein-Protein Interactions by Graphyne. <i>Journal of Physical Chemistry B</i> , 2016, 120, 2124-2131.	1.2	18
49	Nanomechanics of Protein Unfolding Outside a Generic Nanopore. <i>ACS Nano</i> , 2016, 10, 317-323.	7.3	27
50	DNA translocation through single-layer boron nitride nanopores. <i>Soft Matter</i> , 2016, 12, 817-823.	1.2	49
51	Nanopore-Based Sensors for Ligand-Receptor Lead Optimization. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 331-337.	2.1	5
52	Revealing the importance of surface morphology of nanomaterials to biological responses: Adsorption of the villin headpiece onto graphene and phosphorene. <i>Carbon</i> , 2015, 94, 895-902.	5.4	65
53	Simplified TiO2 force fields for studies of its interaction with biomolecules. <i>Journal of Chemical Physics</i> , 2015, 142, 234102.	1.2	41
54	Potential Toxicity of Graphene to Cell Functions <i>via</i> Disrupting Protein-Protein Interactions. <i>ACS Nano</i> , 2015, 9, 663-669.	7.3	164

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55	Controlling the motion of DNA in a nanochannel with transversal alternating electric voltages. <i>Nanotechnology</i> , 2014, 25, 265101.	1.3	4
56	Controlled transport of DNA through a Y-shaped carbon nanotube in a solid membrane. <i>Nanoscale</i> , 2014, 6, 11479-11483.	2.8	11
57	Fabrication of sub-20 nm nanopore arrays in membranes with embedded metal electrodes at wafer scales. <i>Nanoscale</i> , 2014, 6, 8900-8906.	2.8	57
58	Regulating the Transport of DNA through Biofriendly Nanochannels in a Thin Solid Membrane. <i>Scientific Reports</i> , 2014, 4, 3985.	1.6	40
59	An electro-hydrodynamics-based model for the ionic conductivity of solid-state nanopores during DNA translocation. <i>Nanotechnology</i> , 2013, 24, 195702.	1.3	23
60	Fabricatable nanopore sensors with an atomic thickness. <i>Applied Physics Letters</i> , 2013, 103, .	1.5	3
61	End-to-end attraction of duplex DNA. <i>Nucleic Acids Research</i> , 2012, 40, 3812-3821.	6.5	81
62	Dynamics of DNA translocation in a solid-state nanopore immersed in aqueous glycerol. <i>Nanotechnology</i> , 2012, 23, 455102.	1.3	33
63	Nanopore-Based Sensors for Detecting Toxicity of a Carbon Nanotube to Proteins. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2337-2341.	2.1	17
64	Slowing and controlling the translocation of DNA in a solid-state nanopore. <i>Nanoscale</i> , 2012, 4, 1068-1077.	2.8	111
65	Characterizing and Controlling the Motion of ssDNA in a Solid-State Nanopore. <i>Biophysical Journal</i> , 2011, 101, 2214-2222.	0.2	37
66	Electrochemical protection of thin film electrodes in solid state nanopores. <i>Nanotechnology</i> , 2011, 22, 275304.	1.3	22
67	Nanopore-Based DNA Sequencing and DNA Motion Control. , 2011, , 255-286.		2
68	The effect of calcium on the conformation of cobalamin transporter BtuB. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 1153-1162.	1.5	16
69	Control and reversal of the electrophoretic force on DNA in a charged nanopore. <i>Journal of Physics Condensed Matter</i> , 2010, 22, 454123.	0.7	46
70	Tribological Effects on DNA Translocation in a Nanochannel Coated with a Self-Assembled Monolayer. <i>Journal of Physical Chemistry B</i> , 2010, 114, 17172-17176.	1.2	24
71	Electrochemical Characterization of Thin Film Electrodes Toward Developing a DNA Transistor. <i>Langmuir</i> , 2010, 26, 19191-19198.	1.6	21
72	Base-By-Base Ratcheting of Single Stranded DNA through a Solid-State Nanopore. <i>Physical Review Letters</i> , 2010, 104, 238103.	2.9	106

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73	Electric and electrophoretic inversion of the DNA charge in multivalent electrolytes. <i>Soft Matter</i> , 2010, 6, 243-246.	1.2	78
74	Hybrid Atomistic/Continuum Study of Contact and Friction Between Rough Solids. <i>Tribology Letters</i> , 2009, 36, 1-16.	1.2	55
75	Side-by-side And End-to-end Attraction Of Double-stranded DNA. <i>Biophysical Journal</i> , 2009, 96, 578a.	0.2	0
76	Effect of Valence and Concentration of Counterions on Electrophoretic Mobility of DNA in a Solid-State Nanopore. <i>Biophysical Journal</i> , 2009, 96, 648a.	0.2	1
77	In meso crystal structure and docking simulations suggest an alternative proteoglycan binding site in the OpcA outer membrane adhesin. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 71, 24-34.	1.5	40
78	Electro-osmotic screening of the DNA charge in a nanopore. <i>Physical Review E</i> , 2008, 78, 021912.	0.8	142
79	DNA Attraction in Monovalent and Divalent Electrolytes. <i>Journal of the American Chemical Society</i> , 2008, 130, 15754-15755.	6.6	95
80	Strain Softening in Stretched DNA. <i>Physical Review Letters</i> , 2008, 101, 118101.	2.9	42
81	Structure Refinement of the OpcA Adhesin Using Molecular Dynamics. <i>Biophysical Journal</i> , 2007, 93, 3058-3069.	0.2	15
82	Contact of single asperities with varying adhesion: Comparing continuum mechanics to atomistic simulations. <i>Physical Review E</i> , 2006, 74, 026111.	0.8	131
83	The breakdown of continuum models for mechanical contacts. <i>Nature</i> , 2005, 435, 929-932.	13.7	587
84	Multiscale Modeling of Two Dimensional Rough Surface Contacts. <i>Materials Research Society Symposia Proceedings</i> , 2004, 841, R7.4.1.	0.1	3
85	Effect of Inertia and Elasticity on Stick-Slip Motion. <i>Physical Review Letters</i> , 2004, 93, 036105.	2.9	32