

Binquan Luan

List of Publications by Year in descending order

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85
papers

4,062
citations

126858

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123376

61
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95
all docs

95
docs citations

95
times ranked

5699
citing authors

#	ARTICLE	IF	CITATIONS
1	The breakdown of continuum models for mechanical contacts. <i>Nature</i> , 2005, 435, 929-932.	13.7	587
2	Enhanced binding of the N501Y-mutated SARS-CoV-2 spike protein to the human ACE2 receptor: insights from molecular dynamics simulations. <i>FEBS Letters</i> , 2021, 595, 1454-1461.	1.3	165
3	Potential Toxicity of Graphene to Cell Functions via Disrupting Protein-Protein Interactions. <i>ACS Nano</i> , 2015, 9, 663-669.	7.3	164
4	PEGylated graphene oxide elicits strong immunological responses despite surface passivation. <i>Nature Communications</i> , 2017, 8, 14537.	5.8	157
5	Electro-osmotic screening of the DNA charge in a nanopore. <i>Physical Review E</i> , 2008, 78, 021912.	0.8	142
6	Opening Lids: Modulation of Lipase Immobilization by Graphene Oxides. <i>ACS Catalysis</i> , 2016, 6, 4760-4768.	5.5	139
7	Contact of single asperities with varying adhesion: Comparing continuum mechanics to atomistic simulations. <i>Physical Review E</i> , 2006, 74, 026111.	0.8	131
8	In Silico Exploration of the Molecular Mechanism of Clinically Oriented Drugs for Possibly Inhibiting SARS-CoV-2's Main Protease. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 4413-4420.	2.1	118
9	Wettability and friction of water on a MoS2 nanosheet. <i>Applied Physics Letters</i> , 2016, 108, .	1.5	113
10	Slowing and controlling the translocation of DNA in a solid-state nanopore. <i>Nanoscale</i> , 2012, 4, 1068-1077.	2.8	111
11	Base-By-Base Ratcheting of Single Stranded DNA through a Solid-State Nanopore. <i>Physical Review Letters</i> , 2010, 104, 238103.	2.9	106
12	Graphene-Induced Pore Formation on Cell Membranes. <i>Scientific Reports</i> , 2017, 7, 42767.	1.6	103
13	DNA Attraction in Monovalent and Divalent Electrolytes. <i>Journal of the American Chemical Society</i> , 2008, 130, 15754-15755.	6.6	95
14	Complete wetting of graphene by biological lipids. <i>Nanoscale</i> , 2016, 8, 5750-5754.	2.8	83
15	End-to-end attraction of duplex DNA. <i>Nucleic Acids Research</i> , 2012, 40, 3812-3821.	6.5	81
16	Electric and electrophoretic inversion of the DNA charge in multivalent electrolytes. <i>Soft Matter</i> , 2010, 6, 243-246.	1.2	78
17	Targeting Proteases for Treating COVID-19. <i>Journal of Proteome Research</i> , 2020, 19, 4316-4326.	1.8	68
18	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

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19	High-Curvature Nanostructuring Enhances Probe Display for Biomolecular Detection. <i>Nano Letters</i> , 2017, 17, 1289-1295.	4.5	64
20	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
21	Spontaneous Transport of Single-Stranded DNA through Graphene-MoS ₂ Heterostructure Nanopores. <i>ACS Nano</i> , 2018, 12, 3886-3891.	7.3	57
22	Hybrid Atomistic/Continuum Study of Contact and Friction Between Rough Solids. <i>Tribology Letters</i> , 2009, 36, 1-16.	1.2	55
23	DNA translocation through single-layer boron nitride nanopores. <i>Soft Matter</i> , 2016, 12, 817-823.	1.2	49
24	Insights into SARS-CoV-2's Mutations for Evading Human Antibodies: Sacrifice and Survival. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 2820-2826.	2.9	49
25	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
26	Single-File Protein Translocations through Graphene-MoS ₂ Heterostructure Nanopores. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3409-3415.	2.1	45
27	Emerging β -Sheet Rich Conformations in Supercompact Huntingtin Exon-1 Mutant Structures. <i>Journal of the American Chemical Society</i> , 2017, 139, 8820-8827.	6.6	43
28	Strain Softening in Stretched DNA. <i>Physical Review Letters</i> , 2008, 101, 118101.	2.9	42
29	Simplified TiO ₂ force fields for studies of its interaction with biomolecules. <i>Journal of Chemical Physics</i> , 2015, 142, 234102.	1.2	41
30	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
31	Regulating the Transport of DNA through Biofriendly Nanochannels in a Thin Solid Membrane. <i>Scientific Reports</i> , 2014, 4, 3985.	1.6	40
32	Characterizing and Controlling the Motion of ssDNA in a Solid-State Nanopore. <i>Biophysical Journal</i> , 2011, 101, 2214-2222.	0.2	37
33	Spontaneous ssDNA stretching on graphene and hexagonal boron nitride in plane heterostructures. <i>Nature Communications</i> , 2019, 10, 4610.	5.8	36
34	Structure-based lead optimization of herbal medicine rutin for inhibiting SARS-CoV-2's main protease. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25335-25343.	1.3	34
35	Dynamics of DNA translocation in a solid-state nanopore immersed in aqueous glycerol. <i>Nanotechnology</i> , 2012, 23, 455102.	1.3	33
36	Effect of Inertia and Elasticity on Stick-Slip Motion. <i>Physical Review Letters</i> , 2004, 93, 036105.	2.9	32

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37	Membrane Insertion and Phospholipids Extraction by Graphyne Nanosheets. <i>Journal of Physical Chemistry C</i> , 2017, 121, 2444-2450.	1.5	31
38	Combined Computational—Experimental Approach to Explore the Molecular Mechanism of SaCas9 with a Broadened DNA Targeting Range. <i>Journal of the American Chemical Society</i> , 2019, 141, 6545-6552.	6.6	31
39	Atomic-Scale Fluidic Diodes Based on Triangular Nanopores in Bilayer Hexagonal Boron Nitride. <i>Nano Letters</i> , 2019, 19, 977-982.	4.5	31
40	Nanomechanics of Protein Unfolding Outside a Generic Nanopore. <i>ACS Nano</i> , 2016, 10, 317-323.	7.3	27
41	Humidity—Responsive Single—Nanoparticle—Layer Plasmonic Films. <i>Advanced Materials</i> , 2017, 29, 1606796.	11.1	25
42	Detecting Interactions between Nanomaterials and Cell Membranes by Synthetic Nanopores. <i>ACS Nano</i> , 2017, 11, 12615-12623.	7.3	25
43	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
44	Potential disruption of protein-protein interactions by graphene oxide. <i>Journal of Chemical Physics</i> , 2016, 144, 225102.	1.2	24
45	Single Locked Nucleic Acid-Enhanced Nanopore Genetic Discrimination of Pathogenic Serotypes and Cancer Driver Mutations. <i>ACS Nano</i> , 2018, 12, 4194-4205.	7.3	24
46	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
47	Crown Nanopores in Graphene for CO ₂ Capture and Filtration. <i>ACS Nano</i> , 2022, 16, 6274-6281.	7.3	23
48	Electrochemical protection of thin film electrodes in solid state nanopores. <i>Nanotechnology</i> , 2011, 22, 275304.	1.3	22
49	<i>In Silico</i> Antibody Mutagenesis for Optimizing Its Binding to Spike Protein of Severe Acute Respiratory Syndrome Coronavirus 2. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 9781-9787.	2.1	22
50	Understanding interactions between biomolecules and two-dimensional nanomaterials using in silico microscopes. <i>Advanced Drug Delivery Reviews</i> , 2022, 186, 114336.	6.6	22
51	Electrochemical Characterization of Thin Film Electrodes Toward Developing a DNA Transistor. <i>Langmuir</i> , 2010, 26, 19191-19198.	1.6	21
52	Structure—Function Analysis of Resistance to Bamlanivimab by SARS-CoV-2 Variants Kappa, Delta, and Lambda. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5133-5140.	2.5	21
53	Mechanism of Divalent-Ion-Induced Charge Inversion of Bacterial Membranes. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2434-2438.	2.1	20
54	Electrophoretic Transport of Single-Stranded DNA through a Two Dimensional Nanopore Patterned on an In-Plane Heterostructure. <i>ACS Nano</i> , 2020, 14, 13137-13145.	7.3	19

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55	Potential Interference of Protein-Protein Interactions by Graphyne. <i>Journal of Physical Chemistry B</i> , 2016, 120, 2124-2131.	1.2	18
56	A novel self-activation mechanism of <i>Candida antarctica</i> lipase B. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 15709-15714.	1.3	18
57	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
58	Sequential protein unfolding through a carbon nanotube pore. <i>Nanoscale</i> , 2016, 8, 12143-12151.	2.8	17
59	Understanding the graphene quantum dots-ubiquitin interaction by identifying the interaction sites. <i>Carbon</i> , 2017, 121, 285-291.	5.4	17
60	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
61	Structure Refinement of the OpcA Adhesin Using Molecular Dynamics. <i>Biophysical Journal</i> , 2007, 93, 3058-3069.	0.2	15
62	In silico Exploration of Inhibitors for SARS-CoV-2's Papain-Like Protease. <i>Frontiers in Chemistry</i> , 2020, 8, 624163.	1.8	15
63	Stable Cell Clones Harboring Self-Replicating SARS-CoV-2 RNAs for Drug Screen. <i>Journal of Virology</i> , 2022, 96, jvi0221621.	1.5	14
64	Nanopores in Atomically Thin 2D Nanosheets Limit Aqueous Single-Stranded DNA Transport. <i>Physical Review Letters</i> , 2021, 127, 138103.	2.9	13
65	Structural perturbations on huntingtin N17 domain during its folding on 2D-nanomaterials. <i>Nanotechnology</i> , 2017, 28, 354001.	1.3	12
66	Controlled transport of DNA through a Y-shaped carbon nanotube in a solid membrane. <i>Nanoscale</i> , 2014, 6, 11479-11483.	2.8	11
67	Molecular Mechanism of Stabilizing the Helical Structure of Huntingtin N17 in a Micellar Environment. <i>Journal of Physical Chemistry B</i> , 2017, 121, 4713-4721.	1.2	11
68	Parameterization of Molybdenum Disulfide Interacting with Water Using the Free Energy Perturbation Method. <i>Journal of Physical Chemistry B</i> , 2019, 123, 7243-7252.	1.2	11
69	Role of intercalation in the electrical properties of nucleic acids for use in molecular electronics. <i>Nanoscale Horizons</i> , 2021, 6, 651-660.	4.1	10
70	Glassy dynamics in mutant huntingtin proteins. <i>Journal of Chemical Physics</i> , 2018, 149, 072333.	1.2	9
71	Potential interference with microtubule assembly by graphene: a tug-of-war. <i>Nanoscale</i> , 2020, 12, 4968-4974.	2.8	7
72	Nanopore-Based Sensors for Ligand-Receptor Lead Optimization. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 331-337.	2.1	5

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73	Friction and Plasticity in Contacts Between Amorphous Solids. Tribology Letters, 2021, 69, 1.	1.2	5
74	<scp>Crystalâ€structuresâ€guided</scp> design of <scp>fragmentâ€based</scp> drugs for inhibiting the main protease of <scp>SARSâ€CoV</scp>â€2. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1081-1089.	1.5	5
75	Controlling the motion of DNA in a nanochannel with transversal alternating electric voltages. Nanotechnology, 2014, 25, 265101.	1.3	4
76	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
77	Multiscale Modeling of Two Dimensional Rough Surface Contacts. Materials Research Society Symposia Proceedings, 2004, 841, R7.4.1.	0.1	3
78	Fabricatable nanopore sensors with an atomic thickness. Applied Physics Letters, 2013, 103, .	1.5	3
79	Bioâ€nano interactions detected by nanochannel electrophoresis. Electrophoresis, 2016, 37, 2190-2195.	1.3	3
80	Radial dependence of DNA translocation velocity in a solid-state nanopore. Mikrochimica Acta, 2016, 183, 995-1002.	2.5	3
81	Field-Dependent Dehydration and Optimal Ionic Escape Paths for C₂N Membranes. Journal of Physical Chemistry B, 2021, 125, 7044-7059.	1.2	3
82	Energetically stretching proteins on patterned two dimensional nanosheets. Nano Futures, 2020, 4, 035001.	1.0	3
83	Nanopore-Based DNA Sequencing and DNA Motion Control. , 2011, , 255-286.		2
84	Effect of Valence and Concentration of Counterions on Electrophoretic Mobility of DNA in a Solid-State Nanopore. Biophysical Journal, 2009, 96, 648a.	0.2	1
85	Side-by-side And End-to-end Attraction Of Double-stranded DNA. Biophysical Journal, 2009, 96, 578a.	0.2	0