

Guo-Wei Wei

List of Publications by Year in descending order

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125
papers

6,071
citations

61857

43
h-index

91712

69
g-index

139
all docs

139
docs citations

139
times ranked

5628
citing authors

#	ARTICLE	IF	CITATIONS
1	Omicron Variant (B.1.1.529): Infectivity, Vaccine Breakthrough, and Antibody Resistance. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 412-422.	2.5	507
2	Mutations Strengthened SARS-CoV-2 Infectivity. <i>Journal of Molecular Biology</i> , 2020, 432, 5212-5226.	2.0	386
3	TopologyNet: Topology based deep convolutional and multi-task neural networks for biomolecular property predictions. <i>PLoS Computational Biology</i> , 2017, 13, e1005690.	1.5	194
4	Persistent homology analysis of protein structure, flexibility, and folding. <i>International Journal for Numerical Methods in Biomedical Engineering</i> , 2014, 30, 814-844.	1.0	174
5	Representability of algebraic topology for biomolecules in machine learning based scoring and virtual screening. <i>PLoS Computational Biology</i> , 2018, 14, e1005929.	1.5	168
6	Mutations on COVID-19 diagnostic targets. <i>Genomics</i> , 2020, 112, 5204-5213.	1.3	164
7	Vaccine-escape and fast-growing mutations in the United Kingdom, the United States, Singapore, Spain, India, and other COVID-19-devastated countries. <i>Genomics</i> , 2021, 113, 2158-2170.	1.3	164
8	AGL-Score: Algebraic Graph Learning Score for Protein-Ligand Binding Scoring, Ranking, Docking, and Screening. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3291-3304.	2.5	145
9	MIBPB: A software package for electrostatic analysis. <i>Journal of Computational Chemistry</i> , 2011, 32, 756-770.	1.5	127
10	Analysis of SARS-CoV-2 mutations in the United States suggests presence of four substrains and novel variants. <i>Communications Biology</i> , 2021, 4, 228.	2.0	126
11	Quantitative Toxicity Prediction Using Topology Based Multitask Deep Neural Networks. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 520-531.	2.5	116
12	Integration of element specific persistent homology and machine learning for protein-ligand binding affinity prediction. <i>International Journal for Numerical Methods in Biomedical Engineering</i> , 2018, 34, e2914.	1.0	115
13	A topology-based network tree for the prediction of protein-protein binding affinity changes following mutation. <i>Nature Machine Intelligence</i> , 2020, 2, 116-123.	8.3	112
14	Mathematical deep learning for pose and binding affinity prediction and ranking in D3R Grand Challenges. <i>Journal of Computer-Aided Molecular Design</i> , 2019, 33, 71-82.	1.3	106
15	Variational Multiscale Models for Charge Transport. <i>SIAM Review</i> , 2012, 54, 699-754.	4.2	99
16	Differential Geometry Based Multiscale Models. <i>Bulletin of Mathematical Biology</i> , 2010, 72, 1562-1622.	0.9	95
17	Decoding SARS-CoV-2 Transmission and Evolution and Ramifications for COVID-19 Diagnosis, Vaccine, and Medicine. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5853-5865.	2.5	91
18	Prediction and mitigation of mutation threats to COVID-19 vaccines and antibody therapies. <i>Chemical Science</i> , 2021, 12, 6929-6948.	3.7	85

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19	Generative Network Complex for the Automated Generation of Drug-like Molecules. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5682-5698.	2.5	79
20	Omicron BA.2 (B.1.1.529.2): High Potential for Becoming the Next Dominant Variant. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3840-3849.	2.1	79
21	Rigidity Strengthening: A Mechanism for Protein-Ligand Binding. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 1715-1721.	2.5	78
22	Repositioning of 8565 Existing Drugs for COVID-19. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 5373-5382.	2.1	78
23	Are 2D fingerprints still valuable for drug discovery?. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 8373-8390.	1.3	77
24	Algebraic graph-assisted bidirectional transformers for molecular property prediction. <i>Nature Communications</i> , 2021, 12, 3521.	5.8	76
25	Geometric and potential driving formation and evolution of biomolecular surfaces. <i>Journal of Mathematical Biology</i> , 2009, 59, 193-231.	0.8	75
26	Mechanisms of SARS-CoV-2 Evolution Revealing Vaccine-Resistant Mutations in Europe and America. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 11850-11857.	2.1	73
27	Topological Persistent Homology-Based Multi-Task Deep Neural Networks for Simultaneous Predictions of Partition Coefficient and Aqueous Solubility. <i>Journal of Computational Chemistry</i> , 2018, 39, 1444-1454.	1.5	71
28	Multiscale Multiphysics and Multidomain Models of Flexibility and Rigidity. <i>Journal of Chemical Physics</i> , 2013, 139, 194109.	1.2	68
29	Host Immune Response Driving SARS-CoV-2 Evolution. <i>Viruses</i> , 2020, 12, 1095.	1.5	68
30	Boosting Tree-Assisted Multitask Deep Learning for Small Scientific Datasets. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1235-1244.	2.5	66
31	Perspectives on SARS-CoV-2 Main Protease Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 16922-16955.	2.9	63
32	Unveiling the molecular mechanism of SARS-CoV-2 main protease inhibition from 137 crystal structures using algebraic topology and deep learning. <i>Chemical Science</i> , 2020, 11, 12036-12046.	3.7	62
33	Decoding Asymptomatic COVID-19 Infection and Transmission. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 10007-10015.	2.1	61
34	Emerging Vaccine-Breakthrough SARS-CoV-2 Variants. <i>ACS Infectious Diseases</i> , 2022, 8, 546-556.	1.8	59
35	UMAP-assisted K-means clustering of large-scale SARS-CoV-2 mutation datasets. <i>Computers in Biology and Medicine</i> , 2021, 131, 104264.	3.9	57
36	MathDL: mathematical deep learning for D3R Grand Challenge 4. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 131-147.	1.3	56

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37	A review of mathematical representations of biomolecular data. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 4343-4367.	1.3	56
38	Fast and anisotropic flexibility-rigidity index for protein flexibility and fluctuation analysis. <i>Journal of Chemical Physics</i> , 2014, 140, 234105.	1.2	53
39	Multidimensional persistence in biomolecular data. <i>Journal of Computational Chemistry</i> , 2015, 36, 1502-1520.	1.5	53
40	Revealing the Threat of Emerging SARS-CoV-2 Mutations to Antibody Therapies. <i>Journal of Molecular Biology</i> , 2021, 433, 167155.	2.0	53
41	Protein structure prediction beyond AlphaFold. <i>Nature Machine Intelligence</i> , 2019, 1, 336-337.	8.3	52
42	DGGL: Differential geometry-based geometric learning of molecular datasets. <i>International Journal for Numerical Methods in Biomedical Engineering</i> , 2019, 35, e3179.	1.0	52
43	Analysis and prediction of protein folding energy changes upon mutation by element specific persistent homology. <i>Bioinformatics</i> , 2017, 33, 3549-3557.	1.8	48
44	Persistent spectral graph. <i>International Journal for Numerical Methods in Biomedical Engineering</i> , 2020, 36, e3376.	1.0	47
45	GGL-Tox: Geometric Graph Learning for Toxicity Prediction. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 1691-1700.	2.5	43
46	Methodology-Centered Review of Molecular Modeling, Simulation, and Prediction of SARS-CoV-2. <i>Chemical Reviews</i> , 2022, 122, 11287-11368.	23.0	38
47	Topological representations of crystalline compounds for the machine-learning prediction of materials properties. <i>Npj Computational Materials</i> , 2021, 7, .	3.5	36
48	MULTISCALE, MULTIPHYSICS AND MULTIDOMAIN MODELS I: BASIC THEORY. <i>Journal of Theoretical and Computational Chemistry</i> , 2013, 12, 1341006.	1.8	35
49	Object-oriented persistent homology. <i>Journal of Computational Physics</i> , 2016, 305, 276-299.	1.9	34
50	Review of COVID-19 Antibody Therapies. <i>Annual Review of Biophysics</i> , 2021, 50, 1-30.	4.5	34
51	Biomolecular surface construction by PDE transform. <i>International Journal for Numerical Methods in Biomedical Engineering</i> , 2012, 28, 291-316.	1.0	32
52	Multiscale Gaussian network model (mGNM) and multiscale anisotropic network model (mANM). <i>Journal of Chemical Physics</i> , 2015, 143, 204106.	1.2	32
53	Communication: Capturing protein multiscale thermal fluctuations. <i>Journal of Chemical Physics</i> , 2015, 142, 211101.	1.2	31
54	MIB Galerkin method for elliptic interface problems. <i>Journal of Computational and Applied Mathematics</i> , 2014, 272, 195-220.	1.1	30

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55	Cluster learning-assisted directed evolution. <i>Nature Computational Science</i> , 2021, 1, 809-818.	3.8	30
56	ESES: Software for <sc>E</sc>ulerian solvent excluded surface. <i>Journal of Computational Chemistry</i> , 2017, 38, 446-466.	1.5	29
57	Accurate, robust, and reliable calculations of Poisson-Boltzmann binding energies. <i>Journal of Computational Chemistry</i> , 2017, 38, 941-948.	1.5	29
58	Multiscale weighted colored graphs for protein flexibility and rigidity analysis. <i>Journal of Chemical Physics</i> , 2018, 148, 054103.	1.2	29
59	Extracting Predictive Representations from Hundreds of Millions of Molecules. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 10793-10801.	2.1	28
60	Multiresolution persistent homology for excessively large biomolecular datasets. <i>Journal of Chemical Physics</i> , 2015, 143, 134103.	1.2	27
61	Generalized flexibility-rigidity index. <i>Journal of Chemical Physics</i> , 2016, 144, 234106.	1.2	27
62	Feature functional theory-binding predictor (FFT-BP) for the blind prediction of binding free energies. <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	27
63	Persistent topology for cryo-EM data analysis. <i>International Journal for Numerical Methods in Biomedical Engineering</i> , 2015, 31, .	1.0	26
64	Differential geometry based solvation model. III. Quantum formulation. <i>Journal of Chemical Physics</i> , 2011, 135, 194108.	1.2	25
65	Topology-Based Machine Learning Strategy for Cluster Structure Prediction. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 4392-4401.	2.1	25
66	Geometric modeling of subcellular structures, organelles, and multiprotein complexes. <i>International Journal for Numerical Methods in Biomedical Engineering</i> , 2012, 28, 1198-1223.	1.0	24
67	Multiscale geometric modeling of macromolecules I: Cartesian representation. <i>Journal of Computational Physics</i> , 2014, 257, 912-936.	1.9	24
68	Multiresolution Topological Simplification. <i>Journal of Computational Biology</i> , 2015, 22, 887-891.	0.8	24
69	Breaking the polar-nonpolar division in solvation free energy prediction. <i>Journal of Computational Chemistry</i> , 2018, 39, 217-233.	1.5	24
70	Second order method for solving 3D elasticity equations with complex interfaces. <i>Journal of Computational Physics</i> , 2015, 294, 405-438.	1.9	23
71	Protein pocket detection via convex hull surface evolution and associated Reeb graph. <i>Bioinformatics</i> , 2018, 34, i830-i837.	1.8	23
72	Structural cavities are critical to balancing stability and activity of a membrane-integral enzyme. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 22146-22156.	3.3	23

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73	Multiscale geometric modeling of macromolecules II: Lagrangian representation. Journal of Computational Chemistry, 2013, 34, 2100-2120.	1.5	22
74	Quantum dynamics in continuum for proton transport II: Variational solvent-solute interface. International Journal for Numerical Methods in Biomedical Engineering, 2012, 28, 25-51.	1.0	21
75	Parameterization of a geometric flow implicit solvation model. Journal of Computational Chemistry, 2013, 34, 687-695.	1.5	21
76	Quantum dynamics in continuum for proton transport-Generalized correlation. Journal of Chemical Physics, 2012, 136, 134109.	1.2	20
77	Evolutionary de Rham-Hodge method. Discrete and Continuous Dynamical Systems - Series B, 2021, 26, 3785.	0.5	20
78	Automatic parametrization of non-polar implicit solvent models for the blind prediction of solvation free energies. Journal of Chemical Physics, 2016, 145, 124110.	1.2	18
79	A model for genesis of transcription systems. Transcription, 2016, 7, 1-13.	1.7	18
80	Blind prediction of protein B-factor and flexibility. Journal of Chemical Physics, 2018, 149, 134107.	1.2	17
81	Stochastic model for protein flexibility analysis. Physical Review E, 2013, 88, 062709.	0.8	16
82	Molecular nonlinear dynamics and protein thermal uncertainty quantification. Chaos, 2014, 24, 013103.	1.0	16
83	Perspectives on Sharing Models and Related Resources in Computational Biomechanics Research. Journal of Biomechanical Engineering, 2018, 140, .	0.6	16
84	HERMES: Persistent spectral graph software. , 2021, 3, 67.		16
85	A Galerkin formulation of the MIB method for three dimensional elliptic interface problems. Computers and Mathematics With Applications, 2014, 68, 719-745.	1.4	15
86	Matched interface and boundary method for elasticity interface problems. Journal of Computational and Applied Mathematics, 2015, 285, 203-225.	1.1	15
87	Flexibility-rigidity index for protein-nucleic acid flexibility and fluctuation analysis. Journal of Computational Chemistry, 2016, 37, 1283-1295.	1.5	15
88	Generative network complex (GNC) for drug discovery. Communications in Information and Systems, 2019, 19, 241-277.	0.3	14
89	Quantum Dynamics in Continuum for Proton Transport I: Basic Formulation. Communications in Computational Physics, 2013, 13, 285-324.	0.7	13
90	Modeling the Effects of Calcium Overload on Mitochondrial Ultrastructural Remodeling. Applied Sciences (Switzerland), 2021, 11, 2071.	1.3	13

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91	3D hodge decompositions of edge- and face-based vector fields. <i>ACM Transactions on Graphics</i> , 2019, 38, 1-13.	4.9	12
92	The de Rham Hodge Analysis and Modeling of Biomolecules. <i>Bulletin of Mathematical Biology</i> , 2020, 82, 108.	0.9	11
93	Hinge action versus grip in translocation by RNA polymerase. <i>Transcription</i> , 2018, 9, 1-16.	1.7	10
94	Persistent Cohomology for Data With Multicomponent Heterogeneous Information. <i>SIAM Journal on Mathematics of Data Science</i> , 2020, 2, 396-418.	1.0	10
95	Review of applications and challenges of quantitative systems pharmacology modeling and machine learning for heart failure. <i>Journal of Pharmacokinetics and Pharmacodynamics</i> , 2022, 49, 39-50.	0.8	10
96	Aspects of topological approaches for data science. , 2022, 4, 165.		10
97	The impact of surface area, volume, curvature, and Lennard-Jones potential to solvation modeling. <i>Journal of Computational Chemistry</i> , 2017, 38, 24-36.	1.5	9
98	Generative Models for Molecular Design. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5635-5636.	2.5	9
99	Origin of parameter degeneracy and molecular shape relationships in geometric-flow calculations of solvation free energies. <i>Journal of Chemical Physics</i> , 2013, 139, 204108.	1.2	8
100	Proteome-Informed Machine Learning Studies of Cocaine Addiction. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 11122-11134.	2.1	8
101	MLIMC: Machine learning-based implicit-solvent Monte Carlo. <i>Chinese Journal of Chemical Physics</i> , 2021, 34, 683-694.	0.6	8
102	Machine Learning Analysis of Cocaine Addiction Informed by DAT, SERT, and NET-Based Interactome Networks. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2703-2719.	2.3	8
103	Atomic scale design and three-dimensional simulation of ionic diffusive nanofluidic channels. <i>Microfluidics and Nanofluidics</i> , 2015, 19, 665-692.	1.0	7
104	Geometric and electrostatic modeling using molecular rigidity functions. <i>Journal of Computational and Applied Mathematics</i> , 2017, 313, 18-37.	1.1	6
105	Evolutionary homology on coupled dynamical systems with applications to protein flexibility analysis. <i>Journal of Applied and Computational Topology</i> , 2020, 4, 481-507.	1.0	6
106	Atom-specific persistent homology and its application to protein flexibility analysis. <i>Computational and Mathematical Biophysics</i> , 2020, 8, 1-35.	0.6	6
107	Mathematics at the eve of a historic transition in biology. <i>Computational and Mathematical Biophysics</i> , 2017, 5, 138-141.	0.6	3
108	Review of quantitative systems pharmacological modeling in thrombosis. <i>Communications in Information and Systems</i> , 2019, 19, 219-240.	0.3	3

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109	Homotopy continuation for the spectra of persistent Laplacians. , 2021, 3, 677.		2
110	Computational Chemistry in Asia. Journal of Chemical Information and Modeling, 2021, 61, 547-547.	2.5	2
111	AweGNN: Auto-parametrized weighted element-specific graph neural networks for molecules. Computers in Biology and Medicine, 2021, 134, 104460.	3.9	2
112	Charge substitutions at the voltage-sensing module of domain III enhance actions of site-3 and site-4 toxins on an insect sodium channel. Insect Biochemistry and Molecular Biology, 2021, 137, 103625.	1.2	2
113	Divide-and-conquer strategy for large-scale Eulerian solvent excluded surface. Communications in Information and Systems, 2018, 18, 299-329.	0.3	2
114	JCIM Special Issue on Generative Models for Molecular Design. Journal of Chemical Information and Modeling, 2020, 60, 1072-1072.	2.5	1
115	SARS-CoV-2 becoming more infectious as revealed by algebraic topology and deep learning. Communications in Information and Systems, 2021, 21, 31-36.	0.3	1
116	Geometric algebra generation of molecular surfaces. Journal of the Royal Society Interface, 2022, 19, 20220117.	1.5	1
117	Recent Advances in Mathematical Methods for the Analysis of Biomedical Image. International Journal of Biomedical Imaging, 2006, 2006, 1-1.	3.0	0
118	Call for Papers: Special Issue on "Recent Advances in Computational Techniques for Biomedical Imaging" Communications in Numerical Methods in Engineering (CNM). International Journal for Numerical and Analytical Methods in Geomechanics, 2008, 32, 215-215.	1.7	0
119	Call for Papers: Special Issue on "Recent Advances in Computational Techniques for Biomedical Imaging" Communications in Numerical Methods in Engineering (CNM). Numerical Linear Algebra With Applications, 2008, 15, 83-83.	0.9	0
120	Special Issue on "Recent Advances in Computational Techniques for Biomedical Imaging" International Journal for Numerical Methods in Engineering (NME). International Journal for Numerical Methods in Engineering, 2008, 73, 596-596.	1.5	0
121	Call for Papers: Special Issue on "Recent Advances in Computational Techniques for Biomedical Imaging" Communications in Numerical Methods in Engineering (CNM). Communications in Numerical Methods in Engineering, 2008, 24, 83-83.	1.3	0
122	Special Issue on "Recent Advances in Computational Techniques for Biomedical Imaging" International Journal for Numerical Methods in Fluids (FLD). International Journal for Numerical Methods in Fluids, 2008, 56, 467-467.	0.9	0
123	Special issue on recent advances in computational techniques for biomedical imaging. Communications in Numerical Methods in Engineering, 2009, 25, 581-582.	1.3	0
124	Mathematical Methods for Images and Surfaces. International Journal of Biomedical Imaging, 2010, 2010, 1-3.	3.0	0
125	Simulation of Inviscid Compressible Flows Using PDE Transform. Communications in Computational Physics, 2014, 16, 1201-1238.	0.7	0