Zhirong Liu

List of Publications by Year
in descending order

116 papers	6,417 citations	71102 41 h-index	69250 77 g-index
128 all docs	128 docs citations	128 times ranked	7878 citing authors

#	Article	IF	Citations
1	Accurate Single-Molecule Kinetic Isotope Effects. Journal of the American Chemical Society, 2022, , .	13.7	8
2	Structural Amorphization-Induced Topological Order. Physical Review Letters, 2022, 128, 056401.	7.8	26
3	Stochastic Binding Dynamics of a Photoswitchable Single Supramolecular Complex. Advanced Science, 2022, 9, e2200022.	11.2	13
4	Dirac Cones, Elastic Properties, and Carrier Mobility of the FeB₂ Monolayer: The Effects of Symmetry. Journal of Physical Chemistry C, 2022, 126, 617-624.	3.1	7
5	Control of phase ordering and elastic properties in phase field crystals through three-point direct correlation. Physical Review E, 2022, 105, 044802.	2.1	4
6	Dipole-improved gating of azulene-based single-molecule transistors. Journal of Materials Chemistry C, 2022, 10, 7803-7809.	5.5	8
7	The Regulatory Roles of Intrinsically Disordered Linker in VRN1-DNA Phase Separation. International Journal of Molecular Sciences, 2022, 23, 4594.	4.1	2
8	Quantitative Analysis of Dynamic Allostery. Journal of Chemical Information and Modeling, 2022, 62, 2538-2549.	5.4	2
9	More is simpler: Decomposition of <scp>ligandâ€binding</scp> affinity for proteins being disordered. Protein Science, 2022, 31, .	7.6	4
10	Molecular Modeling of Ionic Liquids: Forceâ€Field Validation and Thermodynamic Perspective from Largeâ€Scale Fastâ€Growth Solvation Free Energy Calculations. Advanced Theory and Simulations, 2022, 5, .	2.8	6
11	Reinforcement learning to boost molecular docking upon protein conformational ensemble. Physical Chemistry Chemical Physics, 2021, 23, 6800-6806.	2.8	5
12	Metformin attenuates plaque-associated tau pathology and reduces amyloid-Î² burden in APP/PS1 mice. Alzheimer's Research and Therapy, 2021, 13, 40.	6.2	53
13	The Mechanism of Graphene Vaporâ€“Solid Growth on Insulating Substrates. ACS Nano, 2021, 15, 7399-7408.	14.6	23
14	Allosteric Type and Pathways Are Governed by the Forces of Proteinâ€“Ligand Binding. Journal of Physical Chemistry Letters, 2021, 12, 5404-5412.	4.6	20
15	Theoretical calculation boosting the chemical vapor deposition growth of graphene film. APL Materials, 2021, 9, 060906.	5.1	2
16	Unveiling the full reaction path of the Suzukiâ€“Miyaura cross-coupling in a single-molecule junction. Nature Nanotechnology, 2021, 16, 1214-1223.	31.5	46
17	Charge Segregation in the Intrinsically Disordered Region Governs VRN1 and DNA Liquid-like Phase Separation Robustness. Journal of Molecular Biology, 2021, 433, 167269.	4.2	14
18	BARâ€Based Multiâ€Dimensional Nonequilibrium Pulling for Indirect Construction of QM/MM Free Energy Landscapes: Varying the QM Region. Advanced Theory and Simulations, 2021, 4, 2100185.	2.8	14

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19	Electric fieldâ€“catalyzed single-molecule Diels-Alder reaction dynamics. Science Advances, 2021, 7, .	10.3	51
20	Tunable Symmetry-Breaking-Induced Dual Functions in Stable and Photoswitched Single-Molecule Junctions. Journal of the American Chemical Society, 2021, 143, 20811-20817.	13.7	30
21	A General Picture of Cucurbit[8]uril Hostâ€“Guest Binding. Journal of Chemical Information and Modeling, 2021, 61, 6107-6134.	5.4	35
22	Ensemble-Based Thermodynamics of the Fuzzy Binding between Intrinsically Disordered Proteins and Small-Molecule Ligands. Journal of Chemical Information and Modeling, 2020, 60, 4967-4974.	5.4	7
23	The differential effects of isoflurane and sevoflurane on neonatal mice. Scientific Reports, 2020, 10, 19345.	3.3	15
24	High elastic moduli, controllable bandgap and extraordinary carrier mobility in single-layer diamond. Journal of Materials Chemistry C, 2020, 8, 13819-13826.	5.5	24
25	Interferon Regulatory Factor 5 Mediates Lipopolysaccharide-Induced Neuroinflammation. Frontiers in Immunology, 2020, 11, 600479.	4.8	11
26	Allostery of multidomain proteins with disordered linkers. Current Opinion in Structural Biology, 2020, 62, 175-182.	5.7	28
27	Minimal phase-field crystal modeling of vapor-liquid-solid coexistence and transitions. Physical Review Materials, 2020, 4, .	2.4	6
28	Two-dimensional ferromagnetic-ferroelectric multiferroics in violation of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mi>d</mml:mi><mml:mn>0</mml:mn></mml:msup></mml:m rule. Physical Review B, 2019, 99, .	3.2	60
29	Fluctuation correlations as major determinants of structure- and dynamics-driven allosteric effects. Physical Chemistry Chemical Physics, 2019, 21, 5200-5214.	2.8	14
30	The influence of intrinsic folding mechanism of an unfolded protein on the coupled foldingâ€“binding process during target recognition. Proteins: Structure, Function and Bioinformatics, 2019, 87, 265-275.	2.6	2
31	Carboxylate-Selective Chemical Cross-Linkers for Mass Spectrometric Analysis of Protein Structures. Analytical Chemistry, 2018, 90, 1195-1201.	6.5	42
32	Elastic constants of stressed and unstressed materials in the phase-field crystal model. Physical Review B, 2018, 97, .	3.2	14
33	Spotting the differences in two-dimensional materials â€“ the Raman scattering perspective. Chemical Society Reviews, 2018, 47, 3217-3240.	38.1	71
34	Conservation of Potentially Druggable Cavities in Intrinsically Disordered Proteins. ACS Omega, 2018, 3, 15643-15652.	3.5	22
35	A comprehensive ensemble model for comparing the allosteric effect of ordered and disordered proteins. PLoS Computational Biology, 2018, 14, e1006393.	3.2	17
36	Frontispiece: Reversible Manipulation of Supramolecular Chirality using Host-Guest Dynamics between Î²-Cyclodextrin and Alkyl Amines. Chemistry - A European Journal, 2018, 24, .	3.3	0

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37	Reversible Manipulation of Supramolecular Chirality using Hostâ€“Guest Dynamics between Î²â€Cyclodextrin and Alkyl Amines. Chemistry - A European Journal, 2018, 24, 13734-13739.	3.3	23
38	Angle-adjustable density field formulation for the modeling of crystalline microstructure. Physical Review B, 2018, 97, .	3.2	11
39	Raman Spectra and Strain Effects in Bismuth Oxychalcogenides. Journal of Physical Chemistry C, 2018, 122, 19970-19980.	3.1	76
40	Singular value decomposition for the correlation of atomic fluctuations with arbitrary angle. Proteins: Structure, Function and Bioinformatics, 2018, 86, 1075-1087.	2.6	5
41	Disordered linkers in multidomain allosteric proteins: Entropic effect to favor the open state or enhanced local concentration to favor the closed state?. Protein Science, 2018, 27, 1600-1610.	7.6	25
42	Ultrafast probes of electronâ€“hole transitions between two atomic layers. Nature Communications, 2018, 9, 1859.	12.8	30
43	Stereoelectronic Effect-Induced Conductance Switching in Aromatic Chain Single-Molecule Junctions. Nano Letters, 2017, 17, 856-861.	9.1	76
44	Movement of Dirac points and band gaps in graphyne under rotating strain. Nano Research, 2017, 10, 2005-2020.	10.4	15
45	Controlling the orientations of h-BN during growth on transition metals by chemical vapor deposition. Nanoscale, 2017, 9, 3561-3567.	5.6	32
46	Inâ€Plane Uniaxial Strain in Black Phosphorus Enables the Identification of Crystalline Orientation. Small, 2017, 13, 1700466.	10.0	29
47	Effects of ABCB1, ABCC2, UGT2B7 and HNF4Î± genetic polymorphisms on oxcarbazepine concentrations and therapeutic efficacy in patients with epilepsy. Seizure: the Journal of the British Epilepsy Association, 2017, 51, 102-106.	2.0	24
48	Steering Surface Reaction at Specific Sites with Self-Assembly Strategy. ACS Nano, 2017, 11, 9397-9404.	14.6	38
49	Anisotropic carrier mobility in two-dimensional materials with tilted Dirac cones: theory and application. Physical Chemistry Chemical Physics, 2017, 19, 23942-23950.	2.8	69
50	Monitoring Local Strain Vector in Atomic-Layered MoSe₂ by Second-Harmonic Generation. Nano Letters, 2017, 17, 7539-7543.	9.1	128
51	Scaling Universality between Band Gap and Exciton Binding Energy of Two-Dimensional Semiconductors. Physical Review Letters, 2017, 118, 266401.	7.8	173
52	Dimensions, energetics, and denaturant effects of the protein unstructured state. Protein Science, 2016, 25, 734-747.	7.6	7
53	Substrateâ€Induced Graphene Chemistry for 2D Superlattices with Tunable Periodicities. Advanced Materials, 2016, 28, 2148-2154.	21.0	26
54	Mobility anisotropy of two-dimensional semiconductors. Physical Review B, 2016, 94, .	3.2	198

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55	Raman Spectra and Corresponding Strain Effects in Graphyne and Graphdiyne. Journal of Physical Chemistry C, 2016, 120, 10605-10613.	3.1	116
56	Thermodynamics and kinetics of TopoII action: A consensus on T-segment curvature selection? Comment on â€œDisentangling DNA Moleculesâ€•by Alexander Vologodskii. Physics of Life Reviews, 2016, 18, 135-138.	2.8	1
57	Dimension conversion and scaling of disordered protein chains. Molecular BioSystems, 2016, 12, 2932-2940.	2.9	9
58	Structure-based Inhibitor Design for the Intrinsically Disordered Protein c-Myc. Scientific Reports, 2016, 6, 22298.	3.3	79
59	Covalently bonded single-molecule junctions with stable and reversible photoswitched conductivity. Science, 2016, 352, 1443-1445.	12.6	697
60	Interplay between binding affinity and kinetics in proteinâ€“protein interactions. Proteins: Structure, Function and Bioinformatics, 2016, 84, 920-933.	2.6	11
61	Consistent rationalization of type-2 topoisomerases' unknotting, decatenating, supercoil-relaxing actions and their scaling relation. Journal of Physics Condensed Matter, 2015, 27, 354103.	1.8	7
62	Time-reversal symmetry protected chiral interface states between quantum spin and quantum anomalous Hall insulators. Physical Review B, 2015, 92, .	3.2	17
63	Emergence of a Chern-insulating state from a semi-Dirac dispersion. Physical Review B, 2015, 92, .	3.2	76
64	Spin-1 Dirac-Weyl fermions protected by bipartite symmetry. Journal of Chemical Physics, 2015, 143, 214109.	3.0	11
65	The rare two-dimensional materials with Dirac cones. National Science Review, 2015, 2, 22-39.	9.5	332
66	Binding cavities and druggability of intrinsically disordered proteins. Protein Science, 2015, 24, 688-705.	7.6	41
67	The transition metal surface passivated edges of hexagonal boron nitride (h-BN) and the mechanism of h-BN's chemical vapor deposition (CVD) growth. Physical Chemistry Chemical Physics, 2015, 17, 29327-29334.	2.8	51
68	Intrinsic carrier mobility of Dirac cones: The limitations of deformation potential theory. Journal of Chemical Physics, 2014, 141, 144107.	3.0	32
69	Advantages of proteins being disordered. Protein Science, 2014, 23, 539-550.	7.6	140
70	Identifying spâ€“sp² carbon materials by Raman and infrared spectroscopies. Physical Chemistry Chemical Physics, 2014, 16, 11303-11309.	2.8	81
71	Conductance Switching and Mechanisms in Singleâ€Molecule Junctions. Angewandte Chemie - International Edition, 2013, 52, 8666-8670.	13.8	158
72	Inherent Relationships among Different Biophysical Prediction Methods for Intrinsically Disordered Proteins. Biophysical Journal, 2013, 104, 488-495.	0.5	13

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73	Dirac cones in two-dimensional systems: from hexagonal to square lattices. Physical Chemistry Chemical Physics, 2013, 15, 18855.	2.8	45
74	Evidences for the unfolding mechanism of threeâ€dimensional domain swapping. Protein Science, 2013, 22, 280-286.	7.6	13
75	Comment on â€œStructural and Electronic Properties ofTGraphene: A Two-Dimensional Carbon Allotrope with Tetraringsâ€. Physical Review Letters, 2013, 110, 029603.	7.8	35
76	Graphenequantum dots embedded in a hexagonal BN sheet: identical influences of zigzag/armchair edges. Physical Chemistry Chemical Physics, 2013, 15, 803-806.	2.8	23
77	Bandgap opening in Janus-type mosaic graphene. Journal of Applied Physics, 2013, 113, .	2.5	25
78	Free Radicals: Free Radical Reactions in Two Dimensions: A Case Study on Photochlorination of Graphene (Small 8/2013). Small, 2013, 9, 1387-1387.	10.0	0
79	The existence/absence of Dirac cones in graphynes. New Journal of Physics, 2013, 15, 023004.	2.9	112
80	Widely Tunable Carrier Mobility of Boron Nitrideâ€Embedded Graphene. Small, 2013, 9, 1373-1378.	10.0	53
81	Inverse relationship between carrier mobility and bandgap in graphene. Journal of Chemical Physics, 2013, 138, 084701.	3.0	116
82	Do Intrinsically Disordered Proteins Possess High Specificity in Proteinâ€“Protein Interactions?. Chemistry - A European Journal, 2013, 19, 4462-4467.	3.3	41
83	Identifying Dirac cones in carbon allotropes with square symmetry. Journal of Chemical Physics, 2013, 139, 184701.	3.0	35
84	Ligand Clouds around Protein Clouds: A Scenario of Ligand Binding with Intrinsically Disordered Proteins. PLoS Computational Biology, 2013, 9, e1003249.	3.2	79
85	Binding of Two Intrinsically Disordered Peptides to a Multi-Specific Protein: A Combined Monte Carlo and Molecular Dynamics Study. PLoS Computational Biology, 2012, 8, e1002682.	3.2	37
86	First-principles study of the transport behavior of zigzag graphene nanoribbons tailored by strain. AIP Advances, 2012, 2, .	1.3	20
87	Evolutionary Chlorination of Graphene: From Charge-Transfer Complex to Covalent Bonding and Nonbonding. Journal of Physical Chemistry C, 2012, 116, 844-850.	3.1	94
88	BN-Embedded Graphene with a Ubiquitous Gap Opening. Journal of Physical Chemistry C, 2012, 116, 21098-21103.	3.1	83
89	Threeâ€dimensional domain swapping in the protein structure space. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1610-1619.	2.6	29
90	Cooperativity, Local-Nonlocal Coupling, and Nonnative Interactions: Principles of Protein Folding from Coarse-Grained Models. Annual Review of Physical Chemistry, 2011, 62, 301-326.	10.8	187

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91	Bandgap Opening in Graphene Antidot Lattices: The Missing Half. ACS Nano, 2011, 5, 4023-4030.	14.6	154
92	Theoretical Modeling and Computational Simulation of Electronic Properties of Nanomaterials. Journal of Nanomaterials, 2011, 2011, 1-2.	2.7	0
93	Anchoring Intrinsically Disordered Proteins to Multiple Targets: Lessons from N-Terminus of the p53 Protein. International Journal of Molecular Sciences, 2011, 12, 1410-1430.	4.1	21
94	Strain effects in graphene and graphene nanoribbons: The underlying mechanism. Nano Research, 2010, 3, 545-556.	10.4	170
95	Smoothing molecular interactions: The â€œkinetic bufferâ€•effect of intrinsically disordered proteins. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3251-3259.	2.6	31
96	Optimizing photoelectrochemical properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu chemical codoping. Physical Review B, 2010, 82, .	3.2	62
97	Local site preference rationalizes disentangling by DNA topoisomerases. Physical Review E, 2010, 81, 031902.	2.1	14
98	Folding Simulations of a De Novo Designed Protein with a Î²Î±Î² Fold. Biophysical Journal, 2010, 98, 321-329.	0.5	13
99	Action at Hooked or Twistedâ€“Hooked DNA Juxtapositions Rationalizes Unlinking Preference of Type-2 Topoisomerases. Journal of Molecular Biology, 2010, 400, 963-982.	4.2	27
100	Effects of hydrostatic pressure on Pb(Zr1â^'xTix)O3 near the morphotropic phase boundary. Journal of Applied Physics, 2010, 108, .	2.5	14
101	Spontaneous edge-defect formation and defect-induced conductance suppression in graphene nanoribbons. Physical Review B, 2010, 82, .	3.2	41
102	Nonnative Interactions in Coupled Folding and Binding Processes of Intrinsically Disordered Proteins. PLoS ONE, 2010, 5, e15375.	2.5	36
103	The why and how of DNA unlinking. Nucleic Acids Research, 2009, 37, 661-671.	14.5	164
104	Interplaying roles of native topology and chain length in marginally cooperative and noncooperative folding of small protein fragments. International Journal of Quantum Chemistry, 2009, 109, 3482-3499.	2.0	8
105	Activated dissociation ofO2on Pb(111) surfaces by Pb adatoms. Physical Review B, 2009, 80, .	3.2	7
106	Desolvation Barrier Effects Are a Likely Contributor to the Remarkable Diversity in the Folding Rates of Small Proteins. Journal of Molecular Biology, 2009, 389, 619-636.	4.2	47
107	Kinetic Advantage of Intrinsically Disordered Proteins in Coupled Foldingâ€“Binding Process: A Critical Assessment of the â€œFly-Castingâ€•Mechanism. Journal of Molecular Biology, 2009, 393, 1143-1159.	4.2	246
108	Half metallicity along the edge of zigzag boron nitride nanoribbons. Physical Review B, 2008, 78, .	3.2	226

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109	Efficient chain moves for Monte Carlo simulations of a wormlike DNA model: Excluded volume, supercoils, site juxtapositions, knots, and comparisons with random-flight and lattice models. Journal of Chemical Physics, 2008, 128, 145104.	3.0	28
110	Probing Possible Downhill Folding: Native Contact Topology Likely Places a Significant Constraint on the Folding Cooperativity of Proteins with â^¼40 Residues. Journal of Molecular Biology, 2008, 384, 512-530.	4.2	38
111	Scaling law of the giant Stark effect in boron nitride nanoribbons and nanotubes. Physical Review B, 2008, 78, .	3.2	96
112	Inferring Global Topology from Local Juxtaposition Geometry: Interlinking Polymer Rings and Ramifications for Topoisomerase Action. Biophysical Journal, 2006, 90, 2344-2355.	0.5	35
113	Topological Information Embodied in Local Juxtaposition Geometry Provides a Statistical Mechanical Basis for Unknotting by Type-2 DNA Topoisomerases. Journal of Molecular Biology, 2006, 361, 268-285.	4.2	56
114	Desolvation is a Likely Origin of Robust Enthalpic Barriers to Protein Folding. Journal of Molecular Biology, 2005, 349, 872-889.	4.2	75
115	Chevron Behavior and Isostable Enthalpic Barriers in Protein Folding: Successes and Limitations of Simple GÅ•like Modeling. Biophysical Journal, 2005, 89, 520-535.	0.5	31
116	Solvation and desolvation effects in protein folding: native flexibility, kinetic cooperativity and enthalpic barriers under isostability conditions. Physical Biology, 2005, 2, S75-S85.	1.8	52