

Guanghong Wei

List of Publications by Year in descending order

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141
papers

6,396
citations

53794

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82547

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144
all docs

144
docs citations

144
times ranked

5859
citing authors

#	ARTICLE	IF	CITATIONS
1	Amyloid Oligomers: A Joint Experimental/Computational Perspective on Alzheimer's Disease, Parkinson's Disease, Type II Diabetes, and Amyotrophic Lateral Sclerosis. <i>Chemical Reviews</i> , 2021, 121, 2545-2647.	47.7	406
2	Protein Ensembles: How Does Nature Harness Thermodynamic Fluctuations for Life? The Diverse Functional Roles of Conformational Ensembles in the Cell. <i>Chemical Reviews</i> , 2016, 116, 6516-6551.	47.7	302
3	Probing the Self-Assembly Mechanism of Diphenylalanine-Based Peptide Nanovesicles and Nanotubes. <i>ACS Nano</i> , 2012, 6, 3907-3918.	14.6	264
4	Plugging into Proteins: Poisoning Protein Function by a Hydrophobic Nanoparticle. <i>ACS Nano</i> , 2010, 4, 7508-7514.	14.6	168
5	Carbon Nanotube Inhibits the Formation of β -Sheet-Rich Oligomers of the Alzheimer's Amyloid- β (16-22) Peptide. <i>Biophysical Journal</i> , 2011, 101, 2267-2276.	0.5	168
6	Effects of Solvent on the Structure of the Alzheimer Amyloid- β (25-35) Peptide. <i>Biophysical Journal</i> , 2006, 91, 1638-1647.	0.5	161
7	The molecular mechanism of fullerene-inhibited aggregation of Alzheimer's β -amyloid peptide fragment. <i>Nanoscale</i> , 2014, 6, 9752-9762.	5.6	135
8	Pathway Complexity of Alzheimer's β -Amyloid A β 16-22 Peptide Assembly. <i>Structure</i> , 2004, 12, 1245-1255.	3.3	132
9	Tunable assembly of amyloid-forming peptides into nanosheets as a retrovirus carrier. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 2996-3001.	7.1	123
10	Thermodynamics and dynamics of amyloid peptide oligomerization are sequence dependent. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 75, 954-963.	2.6	114
11	Triphenylalanine peptides self-assemble into nanospheres and nanorods that are different from the nanovesicles and nanotubes formed by diphenylalanine peptides. <i>Nanoscale</i> , 2014, 6, 2800.	5.6	100
12	Complex folding pathways in a simple β -hairpin. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 56, 464-474.	2.6	84
13	Expanding the Nanoarchitectural Diversity Through Aromatic Di- and Tri-Peptide Coassembly: Nanostructures and Molecular Mechanisms. <i>ACS Nano</i> , 2016, 10, 8316-8324.	14.6	84
14	Norepinephrine Inhibits Alzheimer's Amyloid- β Peptide Aggregation and Destabilizes Amyloid- β Protofibrils: A Molecular Dynamics Simulation Study. <i>ACS Chemical Neuroscience</i> , 2019, 10, 1585-1594.	3.5	83
15	Induced β -Barrel Formation of the Alzheimer's A β 25-35 Oligomers on Carbon Nanotube Surfaces: Implication for Amyloid Fibril Inhibition. <i>Biophysical Journal</i> , 2009, 97, 1795-1803.	0.5	82
16	Structural diversity of dimers of the Alzheimer amyloid- β (25-35) peptide and polymorphism of the resulting fibrils. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 3622.	2.8	82
17	Atomic-Level Study of Adsorption, Conformational Change, and Dimerization of an α -Helical Peptide at Graphene Surface. <i>Journal of Physical Chemistry B</i> , 2011, 115, 9813-9822.	2.6	81
18	Structural Insight into Tau Protein's Paradox of Intrinsically Disordered Behavior, Self-Acetylation Activity, and Aggregation. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 3026-3031.	4.6	81

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19	Conformational Ensemble of hIAPP Dimer: Insight into the Molecular Mechanism by which a Green Tea Extract inhibits hIAPP Aggregation. <i>Scientific Reports</i> , 2016, 6, 33076.	3.3	79
20	Self-Assembly of the β 2-Microglobulin NHVTLQ Peptide Using a Coarse-Grained Protein Model Reveals a β -Barrel Species. <i>Journal of Physical Chemistry B</i> , 2008, 112, 4410-4418.	2.6	75
21	Sampling the Self-Assembly Pathways of KFFE Hexamers. <i>Biophysical Journal</i> , 2004, 87, 3648-3656.	0.5	74
22	Unusual Two-Step Assembly of a Minimalistic Dipeptide-Based Functional Hydrogelator. <i>Advanced Materials</i> , 2020, 32, e1906043.	21.0	73
23	Nanoengineered Peptide-Based Antimicrobial Conductive Supramolecular Biomaterial for Cardiac Tissue Engineering. <i>Advanced Materials</i> , 2021, 33, e2008715.	21.0	73
24	Green Tea Extracts EGCG and EGC Display Distinct Mechanisms in Disrupting β 42 Protofibril. <i>ACS Chemical Neuroscience</i> , 2020, 11, 1841-1851.	3.5	73
25	Structural Polymorphism in a Self-Assembled Tri-Aromatic Peptide System. <i>ACS Nano</i> , 2018, 12, 3253-3262.	14.6	72
26	Replica Exchange Molecular Dynamics: A Practical Application Protocol with Solutions to Common Problems and a Peptide Aggregation and Self-Assembly Example. <i>Methods in Molecular Biology</i> , 2018, 1777, 101-119.	0.9	70
27	Conformational Distribution and α -Helix to β -Sheet Transition of Human Amylin Fragment Dimer. <i>Biomacromolecules</i> , 2014, 15, 122-131.	5.4	69
28	Structure and Thermodynamics of Amylin Dimer Studied by Hamiltonian-Temperature Replica Exchange Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2011, 115, 3146-3154.	2.6	67
29	The inhibitory mechanism of a fullerene derivative against amyloid- β peptide aggregation: an atomistic simulation study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 12582-12591.	2.8	67
30	Effect of the Disulfide Bond on the Monomeric Structure of Human Amylin Studied by Combined Hamiltonian and Temperature Replica Exchange Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7071-7077.	2.6	64
31	Conformational Basis for Asymmetric Seeding Barrier in Filaments of Three- and Four-Repeat Tau. <i>Journal of the American Chemical Society</i> , 2012, 134, 10271-10278.	13.7	63
32	Cross-seeding and Conformational Selection between Three- and Four-repeat Human Tau Proteins. <i>Journal of Biological Chemistry</i> , 2012, 287, 14950-14959.	3.4	63
33	Computational Simulations of the Early Steps of Protein Aggregation. <i>Prion</i> , 2007, 1, 3-8.	1.8	62
34	Sampling the complex energy landscape of a simple β -hairpin. <i>Journal of Chemical Physics</i> , 2003, 119, 6403-6406.	3.0	59
35	Expanding the Functional Scope of the Fmoc-Diphenylalanine Hydrogelator by Introducing a Rigidifying and Chemically Active Urea Backbone Modification. <i>Advanced Science</i> , 2019, 6, 1900218.	11.2	57
36	Hydrophobic Interaction Drives Surface-Assisted Epitaxial Assembly of Amyloid-like Peptides. <i>Journal of the American Chemical Society</i> , 2013, 135, 3150-3157.	13.7	56

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37	Influence of Au nanoparticles on the aggregation of amyloid- β -(25-35) peptides. <i>Nanoscale</i> , 2013, 5, 10397.	5.6	54
38	Probing ion channel activity of human islet amyloid polypeptide (amylin). <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2012, 1818, 3121-3130.	2.6	50
39	Sequence Effects on Peptide Assembly Characteristics Observed by Using Scanning Tunneling Microscopy. <i>Journal of the American Chemical Society</i> , 2013, 135, 2181-2187.	13.7	50
40	Interactions of a Water-Soluble Fullerene Derivative with Amyloid- β Protofibrils: Dynamics, Binding Mechanism, and the Resulting Salt-Bridge Disruption. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6733-6741.	2.6	50
41	Interactions of A β ²⁵⁻³⁵ β -Barrel-like Oligomers with Anionic Lipid Bilayer and Resulting Membrane Leakage: An All-Atom Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2011, 115, 1165-1174.	2.6	49
42	The Inhibitory Effect of Hydroxylated Carbon Nanotubes on the Aggregation of Human Islet Amyloid Polypeptide Revealed by a Combined Computational and Experimental Study. <i>ACS Chemical Neuroscience</i> , 2018, 9, 2741-2752.	3.5	49
43	Exploring the energy landscape of proteins: A characterization of the activation-relaxation technique. <i>Journal of Chemical Physics</i> , 2002, 117, 11379-11387.	3.0	48
44	Molecular dynamics simulations reveal the mechanism of graphene oxide nanosheet inhibition of A β ¹⁻⁴² peptide aggregation. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10981-10991.	2.8	48
45	Synergistic Inhibitory Effect of Peptide-Organic Coassemblies on Amyloid Aggregation. <i>ACS Nano</i> , 2016, 10, 4143-4153.	14.6	47
46	Liquid-Liquid Phase Separation of Tau Protein Is Encoded at the Monomeric Level. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2576-2586.	4.6	47
47	Expanding the Structural Diversity and Functional Scope of Diphenylalanine-Based Peptide Architectures by Hierarchical Coassembly. <i>Journal of the American Chemical Society</i> , 2021, 143, 17633-17645.	13.7	47
48	Phase transition of nanotube-confined water driven by electric field. <i>Journal of Chemical Physics</i> , 2011, 134, 154507.	3.0	46
49	Molecular Dynamics Simulations Reveal the Inhibitory Mechanism of Dopamine against Human Islet Amyloid Polypeptide (hIAPP) Aggregation and Its Destabilization Effect on hIAPP Protofibrils. <i>ACS Chemical Neuroscience</i> , 2019, 10, 4151-4159.	3.5	46
50	Structural diversity of the soluble trimers of the human amylin(20-29) peptide revealed by molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2009, 130, 125101.	3.0	44
51	A β ¹⁶⁻²² Peptides Can Assemble into Ordered β -Barrels and Bilayer β -Sheets, while Substitution of Phenylalanine 19 by Tryptophan Increases the Population of Disordered Aggregates. <i>Journal of Physical Chemistry B</i> , 2013, 117, 10149-10160.	2.6	44
52	Lattice dynamics of zinc-blende GaN and AlN: I. Bulk phonons. <i>Journal of Physics Condensed Matter</i> , 1996, 8, 6323-6328.	1.8	42
53	Effects of Hydroxylated Carbon Nanotubes on the Aggregation of A β ¹⁶⁻²² Peptides: A Combined Simulation and Experimental Study. <i>Biophysical Journal</i> , 2014, 107, 1930-1938.	0.5	42
54	A β Stretching-and-Packing-Cross-Seeding Mechanism Can Trigger Tau Protein Aggregation. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 3276-3282.	4.6	42

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55	Self-assembly of amyloid-forming peptides by molecular dynamics simulations. <i>Frontiers in Bioscience - Landmark</i> , 2008, Volume, 5681.	3.0	41
56	Atomic-Level Study of the Effects of O4 Molecules on the Structural Properties of Protofibrillar A β 2 Trimer: β -Sheet Stabilization, Salt Bridge Protection, and Binding Mechanism. <i>Journal of Physical Chemistry B</i> , 2015, 119, 2786-2794.	2.6	40
57	Amphiphilic Peptides A ₆ K and V ₆ K Display Distinct Oligomeric Structures and Self-Assembly Dynamics: A Combined All-Atom and Coarse-Grained Simulation Study. <i>Biomacromolecules</i> , 2015, 16, 2940-2949.	5.4	39
58	Lipid Interaction and Membrane Perturbation of Human Islet Amyloid Polypeptide Monomer and Dimer by Molecular Dynamics Simulations. <i>PLoS ONE</i> , 2012, 7, e38191.	2.5	39
59	Single Mutations in Tau Modulate the Populations of Fibril Conformers through Seed Selection. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 1590-1593.	13.8	38
60	Structural disorder in four-repeat Tau fibrils reveals a new mechanism for barriers to cross-seeding of Tau isoforms. <i>Journal of Biological Chemistry</i> , 2018, 293, 17336-17348.	3.4	35
61	The distinct structural preferences of tau protein repeat domains. <i>Chemical Communications</i> , 2018, 54, 5700-5703.	4.1	35
62	Molecular insights into the reversible formation of tau protein fibrils. <i>Chemical Communications</i> , 2013, 49, 3582.	4.1	34
63	Recent computational studies of membrane interaction and disruption of human islet amyloid polypeptide: Monomers, oligomers and protofibrils. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2018, 1860, 1826-1839.	2.6	34
64	Atomistic-level study of the interactions between hIAPP protofibrils and membranes: Influence of pH and lipid composition. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2018, 1860, 1818-1825.	2.6	33
65	Influence of fulleranol on hIAPP aggregation: amyloid inhibition and mechanistic aspects. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 4022-4031.	2.8	33
66	Prediction and characterization of liquid-liquid phase separation of minimalistic peptides. <i>Cell Reports Physical Science</i> , 2021, 2, 100579.	5.6	33
67	Transformation of an oblate-shaped vesicle induced by an adhering spherical particle. <i>Physical Review E</i> , 2011, 84, 050901.	2.1	32
68	Adsorption and Orientation of Human Islet Amyloid Polypeptide (hIAPP) Monomer at Anionic Lipid Bilayers: Implications for Membrane-Mediated Aggregation. <i>International Journal of Molecular Sciences</i> , 2013, 14, 6241-6258.	4.1	32
69	Binding of protofibrillar A β 2 trimers to lipid bilayer surface enhances A β 2 structural stability and causes membrane thinning. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 27556-27569.	2.8	32
70	Dihydrochalcone molecules destabilize Alzheimer's amyloid- β 2 protofibrils through binding to the protofibril cavity. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 17208-17217.	2.8	32
71	Effects of G33A and G33I Mutations on the Structures of Monomer and Dimer of the Amyloid- β 2 Fragment 29-42 by Replica Exchange Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2011, 115, 1282-1288.	2.6	31
72	Mechanistic insights into the inhibition and size effects of graphene oxide nanosheets on the aggregation of an amyloid- β 2 peptide fragment. <i>Nanoscale</i> , 2018, 10, 8989-8997.	5.6	31

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73	Molecular mechanisms of resveratrol and EGCG in the inhibition of A β ₄₂ aggregation and disruption of A β ₄₂ protofibril: similarities and differences. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 18843-18854.	2.8	31
74	Highly Efficient Destruction of Amyloid- β Fibrils by Femtosecond Laser-Induced Nanoexplosion of Gold Nanorods. <i>ACS Chemical Neuroscience</i> , 2016, 7, 1728-1736.	3.5	30
75	Single-molecule visualization of dynamic transitions of pore-forming peptides among multiple transmembrane positions. <i>Nature Communications</i> , 2016, 7, 12906.	12.8	30
76	Orcein-Related Small Molecule O4 Destabilizes hIAPP Protofibrils by Interacting Mostly with the Amyloidogenic Core Region. <i>Journal of Physical Chemistry B</i> , 2017, 121, 9203-9212.	2.6	30
77	A Comprehensive Insight into the Mechanisms of Dopamine in Disrupting A β Protofibrils and Inhibiting A β Aggregation. <i>ACS Chemical Neuroscience</i> , 2021, 12, 4007-4019.	3.5	28
78	Effects of cholesterol on pore formation in lipid bilayers induced by human islet amyloid polypeptide fragments: A coarse-grained molecular dynamics study. <i>Physical Review E</i> , 2011, 84, 051922.	2.1	27
79	Investigation of the Aggregation Process of Amyloid- β -(16-22) Peptides and the Dissolution of Intermediate Aggregates. <i>Langmuir</i> , 2014, 30, 3170-3175.	3.5	27
80	Zone-center optical phonons in wurtzite GaN and AlN. <i>Journal of Applied Physics</i> , 1997, 82, 4693-4695.	2.5	26
81	Influence of electric fields on the structure and structure transition of water confined in a carbon nanotube. <i>Journal of Chemical Physics</i> , 2014, 140, 154508.	3.0	26
82	Distinct Helix Propensities and Membrane Interactions of Human and Rat IAPP ₁₋₁₉ Monomers in Anionic Lipid Bilayers. <i>Journal of Physical Chemistry B</i> , 2015, 119, 3366-3376.	2.6	26
83	Pristine and Hydroxylated Fullerenes Prevent the Aggregation of Human Islet Amyloid Polypeptide and Display Different Inhibitory Mechanisms. <i>Frontiers in Chemistry</i> , 2020, 8, 51.	3.6	26
84	Epigallocatechin Gallate Destabilizes β -Synuclein Fibril by Disrupting the E46-K80 Salt-Bridge and Inter-protofibril Interface. <i>ACS Chemical Neuroscience</i> , 2020, 11, 4351-4361.	3.5	25
85	Co-Assembly between Fmoc Diphenylalanine and Diphenylalanine within a 3D Fibrous Viscous Network Confers Atypical Curvature and Branching. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 23731-23739.	13.8	25
86	Interaction Dynamics in Inhibiting the Aggregation of A β Peptides by SWCNTs: A Combined Experimental and Coarse-Grained Molecular Dynamic Simulation Study. <i>ACS Chemical Neuroscience</i> , 2016, 7, 1232-1240.	3.5	24
87	Mechanically rigid supramolecular assemblies formed from an Fmoc-guanine conjugated peptide nucleic acid. <i>Nature Communications</i> , 2019, 10, 5256.	12.8	24
88	Serotonin and Melatonin Show Different Modes of Action on A β ₄₂ Protofibril Destabilization. <i>ACS Chemical Neuroscience</i> , 2021, 12, 799-809.	3.5	24
89	Natural stereoisomeric flavonoids exhibit different disruptive effects and the mechanism of action on A β ₄₂ protofibril. <i>Chemical Communications</i> , 2021, 57, 4267-4270.	4.1	24
90	Self-aggregation and coaggregation of the p53 core fragment with its aggregation gatekeeper variant. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 8098-8107.	2.8	23

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91	Mechanistic Insights into the Co-Aggregation of A β 2 and hIAPP: An All-Atom Molecular Dynamic Study. <i>Journal of Physical Chemistry B</i> , 2021, 125, 2050-2060.	2.6	23
92	Conformational stability and dynamics of the cancer-associated isoform β 133p53 β are modulated by p53 peptides and p53-specific DNA. <i>FASEB Journal</i> , 2019, 33, 4225-4235.	0.5	22
93	Critical nucleus of Greek-key-like core of β -synuclein protofibril and its disruption by dopamine and norepinephrine. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 203-211.	2.8	22
94	Structural, thermodynamical, and dynamical properties of oligomers formed by the amyloid NNQQ peptide: Insights from coarse-grained simulations. <i>Journal of Chemical Physics</i> , 2012, 137, 025101.	3.0	21
95	Gate-Controlled Sum-Frequency Vibrational Spectroscopy for Probing Charged Oxide/Water Interfaces. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 5943-5948.	4.6	21
96	Common cancer mutations R175H and R273H drive the p53 DNA-binding domain towards aggregation-prone conformations. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9225-9232.	2.8	21
97	Insights Into the Allosteric Inhibition of the SUMO E2 Enzyme Ubc9. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 5703-5707.	13.8	20
98	Deciphering the Rules for Amino Acid Co-Assembly Based on Interlayer Distances. <i>ACS Nano</i> , 2019, 13, 1703-1712.	14.6	19
99	Green tea extract EGCG plays a dual role in A β 242 protofibril disruption and membrane protection: A molecular dynamic study. <i>Chemistry and Physics of Lipids</i> , 2021, 234, 105024.	3.2	19
100	Conformational dynamics of cancer-associated MyD88-TIR domain mutant L252P (L265P) allosterically tilts the landscape toward homo-dimerization. <i>Protein Engineering, Design and Selection</i> , 2016, 29, 347-354.	2.1	18
101	Mechanistic insight into E22Q-mutation-induced antiparallel-to-parallel β -sheet transition of A β 16-22 fibrils: an all-atom simulation study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 15686-15694.	2.8	18
102	Bioinspired Supramolecular Packing Enables High Thermo-Sustainability. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 19037-19041.	13.8	18
103	Insights into the Atomistic Mechanisms of Phosphorylation in Disrupting Liquid-Liquid Phase Separation and Aggregation of the FUS Low-Complexity Domain. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 3227-3238.	5.4	18
104	Structure and Aggregation Mechanism of β 2-Microglobulin (83-99) Peptides Studied by Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2007, 93, 3353-3362.	0.5	17
105	Membrane Binding and Insertion of a pHILIP Peptide Studied by All-Atom Molecular Dynamics Simulations. <i>International Journal of Molecular Sciences</i> , 2013, 14, 14532-14549.	4.1	16
106	Atomistic mechanisms of huntingtin N-terminal fragment insertion on a phospholipid bilayer revealed by molecular dynamics simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 1409-1427.	2.6	16
107	Electric-Field-Induced Phase Transition of Confined Water Nanofilms between Two Graphene Sheets. <i>Journal of Physical Chemistry A</i> , 2014, 118, 8922-8928.	2.5	16
108	Heparin remodels the microtubule-binding repeat R3 of Tau protein towards fibril-prone conformations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 20406-20418.	2.8	16

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109	All-Atom Stability and Oligomerization Simulations of Polyglutamine Nanotubes with and without the 17-Amino-Acid N-Terminal Fragment of the Huntingtin Protein. <i>Journal of Physical Chemistry B</i> , 2012, 116, 12168-12179.	2.6	15
110	Dynamics of the conformational transitions during the dimerization of an intrinsically disordered peptide: a case study on the human islet amyloid polypeptide fragment. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 29892-29904.	2.8	15
111	Lattice dynamics of GaN/AlN superlattices. <i>Journal of Applied Physics</i> , 1997, 82, 622-627.	2.5	14
112	Expanding the structural diversity of peptide assemblies by coassembling dipeptides with diphenylalanine. <i>Nanoscale</i> , 2020, 12, 3038-3049.	5.6	14
113	Investigation of the Dissociation Mechanism of Single-Walled Carbon Nanotube on Mature Amyloid- β^2 Fibrils at Single Nanotube Level. <i>Journal of Physical Chemistry B</i> , 2020, 124, 3459-3468.	2.6	13
114	Molecular dynamics simulations reveal the destabilization mechanism of Alzheimer's disease-related tau R3-R4 Protofilament by norepinephrine. <i>Biophysical Chemistry</i> , 2021, 271, 106541.	2.8	13
115	The β^2 -Strand-Loop- β^2 -Strand Conformation Is Marginally Populated in β^2 -Microglobulin (20 β^2 41) Peptide in Solution as Revealed by Replica Exchange Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2008, 95, 510-517.	0.5	12
116	Inhibitory effect of hydrophobic fullerenes on the β^2 -sheet-rich oligomers of a hydrophilic GNNQQNY peptide revealed by atomistic simulations. <i>RSC Advances</i> , 2017, 7, 13947-13956.	3.6	12
117	Computational Investigation of Gantenerumab and Crenezumab Recognition of β^2 Fibrils in Alzheimer's Disease Brain Tissue. <i>ACS Chemical Neuroscience</i> , 2020, 11, 3233-3244.	3.5	12
118	Exploring the early steps of aggregation of amyloid-forming peptide KFFE. <i>Journal of Physics Condensed Matter</i> , 2004, 16, S5047-S5054.	1.8	11
119	Lattice dynamics of zinc-blende GaN and AlN: II. Superlattice phonons. <i>Journal of Physics Condensed Matter</i> , 1996, 8, 6329-6336.	1.8	10
120	Carbon nanotube prevents the secondary structure formation of amyloid- β^2 trimers: an all-atom molecular dynamics study. <i>Molecular Simulation</i> , 2017, 43, 1189-1195.	2.0	10
121	Solid-state packing dictates the unexpected solubility of aromatic peptides. <i>Cell Reports Physical Science</i> , 2021, 2, 100391.	5.6	10
122	Unraveling the Allosteric Mechanism of Four Cancer-related Mutations in the Disruption of p53-DNA Interaction. <i>Journal of Physical Chemistry B</i> , 2021, 125, 10138-10148.	2.6	10
123	Binding Orientations and Lipid Interactions of Human Amylin at Zwitterionic and Anionic Lipid Bilayers. <i>Journal of Diabetes Research</i> , 2016, 2016, 1-13.	2.3	9
124	Formation of α -helical and β^2 -sheet structures in membrane-bound human IAPP monomer and the resulting membrane deformation. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 20239-20251.	2.8	9
125	Study on Molecular Cavity of Oligoamide Macrocycles by Using Scanning Tunneling Microscopy. <i>ChemPhysChem</i> , 2012, 13, 3598-3604.	2.1	7
126	Proline hydroxylation at different sites in hypoxia-inducible factor 1α modulates its interactions with the von Hippel-Lindau tumor suppressor protein. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 18756-18765.	2.8	7

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127	ALS-associated A315E and A315pT variants exhibit distinct mechanisms in inducing irreversible aggregation of TDP-43₃₁₂₋₃₁₇ peptides. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 16263-16273.	2.8	6
128	Co-Assembly between Fmoc Diphenylalanine and Diphenylalanine within a 3D Fibrous Viscous Network Confers Atypical Curvature and Branching. <i>Angewandte Chemie</i> , 2020, 132, 23939-23947.	2.0	5
129	Structural and dynamical mechanisms of a naturally occurring variant of the human prion protein in preventing prion conversion. <i>Chinese Physics B</i> , 2020, 29, 108710.	1.4	5
130	Effects of the RGTfEGKF Inhibitor on the Structures of the Transmembrane Fragment 70 [~] 86 of Glycophorin A: An All-Atom Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2010, 114, 1004-1009.	2.6	4
131	Deciphering the mechanisms of HPV E6 mutations in the destabilization of E6/E6AP/p53 complex. <i>Biophysical Journal</i> , 2022, 121, 1704-1714.	0.5	4
132	Dancing with Strings: The Conformational Dynamics of VQIXXX Motifs within Tau Protein in Monomer, Fibril and Hyper-Phosphorylated Filament States. <i>Biophysical Journal</i> , 2016, 110, 553a-554a.	0.5	3
133	Mechanistic insight into the destabilization of p53TD tetramer by cancer-related R337H mutation: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 5199-5210.	2.8	3
134	Editorial overview: Folding and binding: Old concepts, new ideas, novel insights. <i>Current Opinion in Structural Biology</i> , 2015, 30, iv-vi.	5.7	2
135	Bioinspired Supramolecular Packing Enables High Thermo-Sustainability. <i>Angewandte Chemie</i> , 2020, 132, 19199-19203.	2.0	2
136	Insights Into the Allosteric Inhibition of the SUMO E2 Enzyme Ubc9. <i>Angewandte Chemie</i> , 2016, 128, 5797-5801.	2.0	1
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