## Guanghong Wei

List of Publications by Year in descending order

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141 papers 6,396 citations

45 h-index 72 g-index

144 all docs 144 docs citations

times ranked

144

5859 citing authors

#	Article	IF	Citations
1	Mechanistic insight into the destabilization of p53TD tetramer by cancer-related R337H mutation: a molecular dynamics study. Physical Chemistry Chemical Physics, 2022, 24, 5199-5210.	2.8	3
2	Deciphering the mechanisms of HPV E6 mutations in the destabilization of E6/E6AP/p53 complex. Biophysical Journal, 2022, 121, 1704-1714.	0.5	4
3	ALS-associated A315E and A315pT variants exhibit distinct mechanisms in inducing irreversible aggregation of TDP-43 <sub>312â€"317</sub> peptides. Physical Chemistry Chemical Physics, 2022, 24, 16263-16273.	2.8	6
4	Insights into the Atomistic Mechanisms of Phosphorylation in Disrupting Liquid–Liquid Phase Separation and Aggregation of the FUS Low-Complexity Domain. Journal of Chemical Information and Modeling, 2022, 62, 3227-3238.	5.4	18
5	Green tea extract EGCG plays a dual role in $\hat{Al}^2$ 42 protofibril disruption and membrane protection: A molecular dynamic study. Chemistry and Physics of Lipids, 2021, 234, 105024.	3.2	19
6	Heparin remodels the microtubule-binding repeat R3 of Tau protein towards fibril-prone conformations. Physical Chemistry Chemical Physics, 2021, 23, 20406-20418.	2.8	16
7	Serotonin and Melatonin Show Different Modes of Action on $\hat{Al^2}$ sub>42 Protofibril Destabilization. ACS Chemical Neuroscience, 2021, 12, 799-809.	3.5	24
8	Amyloid Oligomers: A Joint Experimental/Computational Perspective on Alzheimer's Disease, Parkinson's Disease, Type II Diabetes, and Amyotrophic Lateral Sclerosis. Chemical Reviews, 2021, 121, 2545-2647.	47.7	406
9	Mechanistic Insights into the Co-Aggregation of ${\rm A\hat{I}^2}$ and hIAPP: An All-Atom Molecular Dynamic Study. Journal of Physical Chemistry B, 2021, 125, 2050-2060.	2.6	23
10	Liquid–Liquid Phase Separation of Tau Protein Is Encoded at the Monomeric Level. Journal of Physical Chemistry Letters, 2021, 12, 2576-2586.	4.6	47
11	Molecular dynamics simulations reveal the destabilization mechanism of Alzheimer's disease-related tau R3-R4 Protofilament by norepinephrine. Biophysical Chemistry, 2021, 271, 106541.	2.8	13
12	Solid-state packing dictates the unexpected solubility of aromatic peptides. Cell Reports Physical Science, 2021, 2, 100391.	5.6	10
13	Nanoengineered Peptideâ€Based Antimicrobial Conductive Supramolecular Biomaterial for Cardiac Tissue Engineering. Advanced Materials, 2021, 33, e2008715.	21.0	<b>7</b> 3
14	Unraveling the Allosteric Mechanism of Four Cancer-related Mutations in the Disruption of p53-DNA Interaction. Journal of Physical Chemistry B, 2021, 125, 10138-10148.	2.6	10
15	A Comprehensive Insight into the Mechanisms of Dopamine in Disrupting AÎ <sup>2</sup> Protofibrils and Inhibiting AÎ <sup>2</sup> Aggregation. ACS Chemical Neuroscience, 2021, 12, 4007-4019.	3.5	28
16	Prediction and characterization of liquid-liquid phase separation of minimalistic peptides. Cell Reports Physical Science, 2021, 2, 100579.	5.6	33
17	Natural stereoisomeric flavonoids exhibit different disruptive effects and the mechanism of action on Al $^2$ < sub > 42 < /sub > protofibril. Chemical Communications, 2021, 57, 4267-4270.	4.1	24
18	Molecular mechanisms of resveratrol and EGCG in the inhibition of $A\hat{l}^2$ <sub>42</sub> aggregation and disruption of $A\hat{l}^2$ <sub>42</sub> protofibril: similarities and differences. Physical Chemistry Chemical Physics, 2021, 23, 18843-18854.	2.8	31

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19	Expanding the Structural Diversity and Functional Scope of Diphenylalanine-Based Peptide Architectures by Hierarchical Coassembly. Journal of the American Chemical Society, 2021, 143, 17633-17645.	13.7	47
20	Critical nucleus of Greek-key-like core of α-synuclein protofibril and its disruption by dopamine and norepinephrine. Physical Chemistry Chemical Physics, 2020, 22, 203-211.	2.8	22
21	Bioinspired Supramolecular Packing Enables High Thermoâ€Sustainability. Angewandte Chemie - International Edition, 2020, 59, 19037-19041.	13.8	18
22	Epigallocatechin Gallate Destabilizes α-Synuclein Fibril by Disrupting the E46–K80 Salt-Bridge and Inter-protofibril Interface. ACS Chemical Neuroscience, 2020, 11, 4351-4361.	3.5	25
23	Bioinspired Supramolecular Packing Enables High Thermoâ€Sustainability. Angewandte Chemie, 2020, 132, 19199-19203.	2.0	2
24	Computational Investigation of Gantenerumab and Crenezumab Recognition of Aβ Fibrils in Alzheimer's Disease Brain Tissue. ACS Chemical Neuroscience, 2020, 11, 3233-3244.	3.5	12
25	Coâ€Assembly between Fmoc Diphenylalanine and Diphenylalanine within a 3D Fibrous Viscous Network Confers Atypical Curvature and Branching. Angewandte Chemie - International Edition, 2020, 59, 23731-23739.	13.8	25
26	Coâ€Assembly between Fmoc Diphenylalanine and Diphenylalanine within a 3D Fibrous Viscous Network Confers Atypical Curvature and Branching. Angewandte Chemie, 2020, 132, 23939-23947.	2.0	5
27	Common cancer mutations R175H and R273H drive the p53 DNA-binding domain towards aggregation-prone conformations. Physical Chemistry Chemical Physics, 2020, 22, 9225-9232.	2.8	21
28	Pristine and Hydroxylated Fullerenes Prevent the Aggregation of Human Islet Amyloid Polypeptide and Display Different Inhibitory Mechanisms. Frontiers in Chemistry, 2020, 8, 51.	3.6	26
29	Unusual Twoâ€Step Assembly of a Minimalistic Dipeptideâ€Based Functional Hypergelator. Advanced Materials, 2020, 32, e1906043.	21.0	73
30	Expanding the structural diversity of peptide assemblies by coassembling dipeptides with diphenylalanine. Nanoscale, 2020, 12, 3038-3049.	5.6	14
31	Investigation of the Dissociation Mechanism of Single-Walled Carbon Nanotube on Mature Amyloid-Î <sup>2</sup> Fibrils at Single Nanotube Level. Journal of Physical Chemistry B, 2020, 124, 3459-3468.	2.6	13
32	Green Tea Extracts EGCG and EGC Display Distinct Mechanisms in Disrupting AÎ <sup>2</sup> <sub>42</sub> Protofibril. ACS Chemical Neuroscience, 2020, 11, 1841-1851.	3.5	73
33	Structural and dynamical mechanisms of a naturally occurring variant of the human prion protein in preventing prion conversion. Chinese Physics B, 2020, 29, 108710.	1.4	5
34	Mechanistic insight into E22Q-mutation-induced antiparallel-to-parallel $\hat{l}^2$ -sheet transition of $A\hat{l}^2$ <sub><math>16\hat{a}^2</math>2</sub> fibrils: an all-atom simulation study. Physical Chemistry Chemical Physics, 2019, 21, 15686-15694.	2.8	18
35	Gate-Controlled Sum-Frequency Vibrational Spectroscopy for Probing Charged Oxide/Water Interfaces. Journal of Physical Chemistry Letters, 2019, 10, 5943-5948.	4.6	21
36	Molecular Dynamics Simulations Reveal the Inhibitory Mechanism of Dopamine against Human Islet Amyloid Polypeptide (hIAPP) Aggregation and Its Destabilization Effect on hIAPP Protofibrils. ACS Chemical Neuroscience, 2019, 10, 4151-4159.	3 <b>.</b> 5	46

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37	Formation of $\hat{l}$ ±-helical and $\hat{l}^2$ -sheet structures in membrane-bound human IAPP monomer and the resulting membrane deformation. Physical Chemistry Chemical Physics, 2019, 21, 20239-20251.	2.8	9
38	Deciphering the Rules for Amino Acid Co-Assembly Based on Interlayer Distances. ACS Nano, 2019, 13, 1703-1712.	14.6	19
39	Influence of fullerenol on hIAPP aggregation: amyloid inhibition and mechanistic aspects. Physical Chemistry Chemical Physics, 2019, 21, 4022-4031.	2.8	33
40	Molecular dynamics simulations reveal the mechanism of graphene oxide nanosheet inhibition of Aβ <sub>1–42</sub> peptide aggregation. Physical Chemistry Chemical Physics, 2019, 21, 10981-10991.	2.8	48
41	Expanding the Functional Scope of the Fmocâ€Diphenylalanine Hydrogelator by Introducing a Rigidifying and Chemically Active Urea Backbone Modification. Advanced Science, 2019, 6, 1900218.	11.2	57
42	Mechanically rigid supramolecular assemblies formed from an Fmoc-guanine conjugated peptide nucleic acid. Nature Communications, 2019, 10, 5256.	12.8	24
43	Norepinephrine Inhibits Alzheimer's Amyloid-β Peptide Aggregation and Destabilizes Amyloid-β Protofibrils: A Molecular Dynamics Simulation Study. ACS Chemical Neuroscience, 2019, 10, 1585-1594.	3.5	83
44	Conformational stability and dynamics of the cancerâ€associated isoform Δ133p53β are modulated by p53 peptides and p53â€specific DNA. FASEB Journal, 2019, 33, 4225-4235.	0.5	22
45	Mechanistic insights into the inhibition and size effects of graphene oxide nanosheets on the aggregation of an amyloid- $\hat{l}^2$ peptide fragment. Nanoscale, 2018, 10, 8989-8997.	5.6	31
46	Atomistic-level study of the interactions between hIAPP protofibrils and membranes: Influence of pH and lipid composition. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 1818-1825.	2.6	33
47	Recent computational studies of membrane interaction and disruption of human islet amyloid polypeptide: Monomers, oligomers and protofibrils. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 1826-1839.	2.6	34
48	Structural Polymorphism in a Self-Assembled Tri-Aromatic Peptide System. ACS Nano, 2018, 12, 3253-3262.	14.6	72
49	Structural disorder in four-repeat Tau fibrils reveals a new mechanism for barriers to cross-seeding of Tau isoforms. Journal of Biological Chemistry, 2018, 293, 17336-17348.	3.4	35
50	Dihydrochalcone molecules destabilize Alzheimer's amyloid- $\hat{l}^2$ protofibrils through binding to the protofibril cavity. Physical Chemistry Chemical Physics, 2018, 20, 17208-17217.	2.8	32
51	Proline hydroxylation at different sites in hypoxia-inducible factor 1α modulates its interactions with the von Hippel–Lindau tumor suppressor protein. Physical Chemistry Chemical Physics, 2018, 20, 18756-18765.	2.8	7
52	The Inhibitory Effect of Hydroxylated Carbon Nanotubes on the Aggregation of Human Islet Amyloid Polypeptide Revealed by a Combined Computational and Experimental Study. ACS Chemical Neuroscience, 2018, 9, 2741-2752.	3.5	49
53	The distinct structural preferences of tau protein repeat domains. Chemical Communications, 2018, 54, 5700-5703.	4.1	35
54	Replica Exchange Molecular Dynamics: A Practical Application Protocol with Solutions to Common Problems and a Peptide Aggregation and Self-Assembly Example. Methods in Molecular Biology, 2018, 1777, 101-119.	0.9	70

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55	Self-Assembling ABETA(30-36) Peptides: A Combined All-Atom and Coarse-Grained Simulation Study. Biophysical Journal, 2018, 114, 229a.	0.5	O
56	Inhibitory effect of hydrophobic fullerenes on the $\hat{l}^2$ -sheet-rich oligomers of a hydrophilic GNNQQNY peptide revealed by atomistic simulations. RSC Advances, 2017, 7, 13947-13956.	3.6	12
57	Carbon nanotube prevents the secondary structure formation of amyloid- $\hat{l}^2$ trimers: an all-atom molecular dynamics study. Molecular Simulation, 2017, 43, 1189-1195.	2.0	10
58	Exploring the Aggregation Mechanism of Intrinsically Disordered Tau Protein. World Scientific Lecture and Course Notes in Chemistry, 2017, , 51-71.	0.2	1
59	Binding of protofibrillar $\hat{Al^2}$ trimers to lipid bilayer surface enhances $\hat{Al^2}$ structural stability and causes membrane thinning. Physical Chemistry Chemical Physics, 2017, 19, 27556-27569.	2.8	32
60	Orcein-Related Small Molecule O4 Destabilizes hIAPP Protofibrils by Interacting Mostly with the Amyloidogenic Core Region. Journal of Physical Chemistry B, 2017, 121, 9203-9212.	2.6	30
61	Binding Orientations and Lipid Interactions of Human Amylin at Zwitterionic and Anionic Lipid Bilayers. Journal of Diabetes Research, 2016, 2016, 1-13.	2.3	9
62	Insights Into the Allosteric Inhibition of the SUMO E2 Enzyme Ubc9. Angewandte Chemie, 2016, 128, 5797-5801.	2.0	1
63	The inhibitory mechanism of a fullerene derivative against amyloid- $\hat{l}^2$ peptide aggregation: an atomistic simulation study. Physical Chemistry Chemical Physics, 2016, 18, 12582-12591.	2.8	67
64	Dynamics of the conformational transitions during the dimerization of an intrinsically disordered peptide: a case study on the human islet amyloid polypeptide fragment. Physical Chemistry Chemical Physics, 2016, 18, 29892-29904.	2.8	15
65	Conformational dynamics of cancer-associated MyD88-TIR domain mutant L252P (L265P) allosterically tilts the landscape toward homo-dimerization. Protein Engineering, Design and Selection, 2016, 29, 347-354.	2.1	18
66	Expanding the Nanoarchitectural Diversity Through Aromatic Di- and Tri-Peptide Coassembly: Nanostructures and Molecular Mechanisms. ACS Nano, 2016, 10, 8316-8324.	14.6	84
67	Highly Efficient Destruction of Amyloid- $\hat{l}^2$ Fibrils by Femtosecond Laser-Induced Nanoexplosion of Gold Nanorods. ACS Chemical Neuroscience, 2016, 7, 1728-1736.	3 <b>.</b> 5	30
68	Interaction Dynamics in Inhibiting the Aggregation of $\hat{A^2}$ Peptides by SWCNTs: A Combined Experimental and Coarse-Grained Molecular Dynamic Simulation Study. ACS Chemical Neuroscience, 2016, 7, 1232-1240.	<b>3.</b> 5	24
69	Single-molecule visualization of dynamic transitions of pore-forming peptides among multiple transmembrane positions. Nature Communications, 2016, 7, 12906.	12.8	30
70	Conformational Ensemble of hIAPP Dimer: Insight into the Molecular Mechanism by which a Green Tea Extract inhibits hIAPP Aggregation. Scientific Reports, 2016, 6, 33076.	3.3	79
71	Insights Into the Allosteric Inhibition of the SUMO E2 Enzyme Ubc9. Angewandte Chemie - International Edition, 2016, 55, 5703-5707.	13.8	20
72	Dancing with Strings: The Conformational Dynamics of VQIXXK Motifs within Tau Protein in Monomer, Fibril and Hyper-Phosphorylated Filament States. Biophysical Journal, 2016, 110, 553a-554a.	0.5	3

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73	Protein Ensembles: How Does Nature Harness Thermodynamic Fluctuations for Life? The Diverse Functional Roles of Conformational Ensembles in the Cell. Chemical Reviews, 2016, 116, 6516-6551.	47.7	302
74	Synergistic Inhibitory Effect of Peptide–Organic Coassemblies on Amyloid Aggregation. ACS Nano, 2016, 10, 4143-4153.	14.6	47
75	Self-aggregation and coaggregation of the p53 core fragment with its aggregation gatekeeper variant. Physical Chemistry Chemical Physics, 2016, 18, 8098-8107.	2.8	23
76	Distinct Helix Propensities and Membrane Interactions of Human and Rat IAPP <sub>1â€"19</sub> Monomers in Anionic Lipid Bilayers. Journal of Physical Chemistry B, 2015, 119, 3366-3376.	2.6	26
77	Atomic-Level Study of the Effects of O4 Molecules on the Structural Properties of Protofibrillar $\hat{A}^2$ Trimer: $\hat{I}^2$ -Sheet Stabilization, Salt Bridge Protection, and Binding Mechanism. Journal of Physical Chemistry B, 2015, 119, 2786-2794.	2.6	40
78	Tunable assembly of amyloid-forming peptides into nanosheets as a retrovirus carrier. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 2996-3001.	7.1	123
79	Aβ "Stretching-and-Packing―Cross-Seeding Mechanism Can Trigger Tau Protein Aggregation. Journal of Physical Chemistry Letters, 2015, 6, 3276-3282.	4.6	42
80	Editorial overview: Folding and binding: Old concepts, new ideas, novel insights. Current Opinion in Structural Biology, 2015, 30, iv-vi.	5.7	2
81	Effects of Carbon Nanoparticles on the Aggregation of Alzheimers Beta-Amyloid Peptide. Biophysical Journal, 2015, 108, 66a-67a.	0.5	0
82	Amphiphilic Peptides A <sub>6</sub> K and V <sub>6</sub> K Display Distinct Oligomeric Structures and Self-Assembly Dynamics: A Combined All-Atom and Coarse-Grained Simulation Study. Biomacromolecules, 2015, 16, 2940-2949.	5.4	39
83	Influence of electric fields on the structure and structure transition of water confined in a carbon nanotube. Journal of Chemical Physics, 2014, 140, 154508.	3.0	26
84	Investigation of the Aggregation Process of Amyloid- $\hat{l}^2$ -(16-22) Peptides and the Dissolution of Intermediate Aggregates. Langmuir, 2014, 30, 3170-3175.	3.5	27
85	Conformational Distribution and $\hat{l}_{\pm}$ -Helix to $\hat{l}^2$ -Sheet Transition of Human Amylin Fragment Dimer. Biomacromolecules, 2014, 15, 122-131.	5.4	69
86	Effects of Hydroxylated Carbon Nanotubes on the Aggregation of A β 16–22 Peptides: A Combined Simulation and Experimental Study. Biophysical Journal, 2014, 107, 1930-1938.	0.5	42
87	Structural Insight into Tau Protein's Paradox of Intrinsically Disordered Behavior, Self-Acetylation Activity, and Aggregation. Journal of Physical Chemistry Letters, 2014, 5, 3026-3031.	4.6	81
88	Atomistic mechanisms of huntingtin Nâ€terminal fragment insertion on a phospholipid bilayer revealed by molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1409-1427.	2.6	16
89	The molecular mechanism of fullerene-inhibited aggregation of Alzheimer's $\hat{l}^2$ -amyloid peptide fragment. Nanoscale, 2014, 6, 9752-9762.	5 <b>.</b> 6	135
90	Triphenylalanine peptides self-assemble into nanospheres and nanorods that are different from the nanovesicles and nanotubes formed by diphenylalanine peptides. Nanoscale, 2014, 6, 2800.	5.6	100

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91	Interactions of a Water-Soluble Fullerene Derivative with Amyloid- $\hat{l}^2$ Protofibrils: Dynamics, Binding Mechanism, and the Resulting Salt-Bridge Disruption. Journal of Physical Chemistry B, 2014, 118, 6733-6741.	2.6	50
92	Electric-Field-Induced Phase Transition of Confined Water Nanofilms between Two Graphene Sheets. Journal of Physical Chemistry A, 2014, 118, 8922-8928.	2.5	16
93	Single Mutations in Tau Modulate the Populations of Fibril Conformers through Seed Selection. Angewandte Chemie - International Edition, 2014, 53, 1590-1593.	13.8	38
94	Membrane Binding and Insertion of a pHLIP Peptide Studied by All-Atom Molecular Dynamics Simulations. International Journal of Molecular Sciences, 2013, 14, 14532-14549.	4.1	16
95	Aβ(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. Journal of Physical Chemistry B, 2013, 117, 10149-10160.	2.6	44
96	Influence of Au nanoparticles on the aggregation of amyloid-β-(25–35) peptides. Nanoscale, 2013, 5, 10397.	5.6	54
97	Molecular insights into the reversible formation of tau protein fibrils. Chemical Communications, 2013, 49, 3582.	4.1	34
98	Sequence Effects on Peptide Assembly Characteristics Observed by Using Scanning Tunneling Microscopy. Journal of the American Chemical Society, 2013, 135, 2181-2187.	13.7	50
99	Hydrophobic Interaction Drives Surface-Assisted Epitaxial Assembly of Amyloid-like Peptides. Journal of the American Chemical Society, 2013, 135, 3150-3157.	13.7	56
100	Adsorption and Orientation of Human Islet Amyloid Polypeptide (hIAPP) Monomer at Anionic Lipid Bilayers: Implications for Membrane-Mediated Aggregation. International Journal of Molecular Sciences, 2013, 14, 6241-6258.	4.1	32
101	STRUCTURAL INSIGHT INTO THE POLYMORPHISM OF NNQNTF PROTOFIBRIL: IMPORTANCE OF INTERFACIAL WATER, POLAR AND AROMATIC RESIDUES. Journal of Theoretical and Computational Chemistry, 2013, 12, 1341012.	1.8	0
102	Structural, thermodynamical, and dynamical properties of oligomers formed by the amyloid NNQQ peptide: Insights from coarse-grained simulations. Journal of Chemical Physics, 2012, 137, 025101.	3.0	21
103	Conformational Basis for Asymmetric Seeding Barrier in Filaments of Three- and Four-Repeat Tau. Journal of the American Chemical Society, 2012, 134, 10271-10278.	13.7	63
104	Probing the Self-Assembly Mechanism of Diphenylalanine-Based Peptide Nanovesicles and Nanotubes. ACS Nano, 2012, 6, 3907-3918.	14.6	264
105	Study on Molecular Cavity of Oligoamide Macrocycles by Using Scanning Tunneling Microscopy. ChemPhysChem, 2012, 13, 3598-3604.	2.1	7
106	All-Atom Stability and Oligomerization Simulations of Polyglutamine Nanotubes with and without the 17-Amino-Acid N-Terminal Fragment of the Huntingtin Protein. Journal of Physical Chemistry B, 2012, 116, 12168-12179.	2.6	15
107	Probing ion channel activity of human islet amyloid polypeptide (amylin). Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 3121-3130.	2.6	50
108	Multiscale Simulation of Polyglutamine and the Effect of Neighboring Amino Acids on Oligomerization. Biophysical Journal, 2012, 102, 733a.	0.5	0

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109	Cross-seeding and Conformational Selection between Three- and Four-repeat Human Tau Proteins. Journal of Biological Chemistry, 2012, 287, 14950-14959.	3.4	63
110	Lipid Interaction and Membrane Perturbation of Human Islet Amyloid Polypeptide Monomer and Dimer by Molecular Dynamics Simulations. PLoS ONE, 2012, 7, e38191.	2.5	39
111	Effects of G33A and G33I Mutations on the Structures of Monomer and Dimer of the Amyloid- $\hat{l}^2$ Fragment 29â°'42 by Replica Exchange Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 1282-1288.	2.6	31
112	Structure and Thermodynamics of Amylin Dimer Studied by Hamiltonian-Temperature Replica Exchange Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 3146-3154.	2.6	67
113	Carbon Nanotube Inhibits the Formation of $\hat{l}^2$ -Sheet-Rich Oligomers of the Alzheimer's Amyloid- $\hat{l}^2$ (16-22) Peptide. Biophysical Journal, 2011, 101, 2267-2276.	0.5	168
114	Interactions of Al $^2$ 25a $^{\circ}$ 35 l $^2$ -Barrel-like Oligomers with Anionic Lipid Bilayer and Resulting Membrane Leakage: An All-Atom Molecular Dynamics Study. Journal of Physical Chemistry B, 2011, 115, 1165-1174.	2.6	49
115	Atomic-Level Study of Adsorption, Conformational Change, and Dimerization of an α-Helical Peptide at Graphene Surface. Journal of Physical Chemistry B, 2011, 115, 9813-9822.	2.6	81
116	Phase transition of nanotube-confined water driven by electric field. Journal of Chemical Physics, 2011, 134, 154507.	3.0	46
117	Effects of cholesterol on pore formation in lipid bilayers induced by human islet amyloid polypeptide fragments: A coarse-grained molecular dynamics study. Physical Review E, 2011, 84, 051922.	2.1	27
118	Transformation of an oblate-shaped vesicle induced by an adhering spherical particle. Physical Review E, 2011, 84, 050901.	2.1	32
119	Structural diversity of dimers of the Alzheimer amyloid-β(25–35) peptide and polymorphism of the resulting fibrils. Physical Chemistry Chemical Physics, 2010, 12, 3622.	2.8	82
120	Plugging into Proteins: Poisoning Protein Function by a Hydrophobic Nanoparticle. ACS Nano, 2010, 4, 7508-7514.	14.6	168
121	Effects of the RGTFEGKF Inhibitor on the Structures of the Transmembrane Fragment 70â^86 of Glycophorin A: An All-Atom Molecular Dynamics Study. Journal of Physical Chemistry B, 2010, 114, 1004-1009.	2.6	4
122	Effect of the Disulfide Bond on the Monomeric Structure of Human Amylin Studied by Combined Hamiltonian and Temperature Replica Exchange Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 7071-7077.	2.6	64
123	Structural diversity of the soluble trimers of the human amylin(20–29) peptide revealed by molecular dynamics simulations. Journal of Chemical Physics, 2009, 130, 125101.	3.0	44
124	Thermodynamics and dynamics of amyloid peptide oligomerization are sequence dependent. Proteins: Structure, Function and Bioinformatics, 2009, 75, 954-963.	2.6	114
125	Induced β-Barrel Formation of the Alzheimer's Aβ25–35 Oligomers on Carbon Nanotube Surfaces: Implication for Amyloid Fibril Inhibition. Biophysical Journal, 2009, 97, 1795-1803.	0.5	82
126	The β-Strand-Loop-β-Strand Conformation Is Marginally Populated in β2-Microglobulin (20–41) Peptide in Solution as Revealed by Replica Exchange Molecular Dynamics Simulations. Biophysical Journal, 2008, 95, 510-517.	0.5	12

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127	Self-Assembly of the $\hat{I}^2$ 2-Microglobulin NHVTLSQ Peptide Using a Coarse-Grained Protein Model Reveals a $\hat{I}^2$ -Barrel Species. Journal of Physical Chemistry B, 2008, 112, 4410-4418.	2.6	75
128	Self-assembly of amyloid-forming peptides by molecular dynamics simulations. Frontiers in Bioscience - Landmark, 2008, Volume, 5681.	3.0	41
129	Computational Simulations of the Early Steps of Protein Aggregation. Prion, 2007, 1, 3-8.	1.8	62
130	Structure and Aggregation Mechanism of β2-Microglobulin (83–99) Peptides Studied by Molecular Dynamics Simulations. Biophysical Journal, 2007, 93, 3353-3362.	0.5	17
131	Effects of Solvent on the Structure of the Alzheimer Amyloid-β(25–35) Peptide. Biophysical Journal, 2006, 91, 1638-1647.	0.5	161
132	Exploring the early steps of aggregation of amyloid-forming peptide KFFE. Journal of Physics Condensed Matter, 2004, 16, S5047-S5054.	1.8	11
133	Pathway Complexity of Alzheimer's $\hat{l}^2$ -Amyloid A $\hat{l}^2$ 16-22 Peptide Assembly. Structure, 2004, 12, 1245-1255.	3.3	132
134	Complex folding pathways in a simple $\hat{l}^2$ -hairpin. Proteins: Structure, Function and Bioinformatics, 2004, 56, 464-474.	2.6	84
135	Sampling the Self-Assembly Pathways of KFFE Hexamers. Biophysical Journal, 2004, 87, 3648-3656.	0.5	74
136	Sampling the complex energy landscape of a simple $\hat{l}^2$ -hairpin. Journal of Chemical Physics, 2003, 119, 6403-6406.	3.0	59
137	Exploring the energy landscape of proteins: A characterization of the activation-relaxation technique. Journal of Chemical Physics, 2002, 117, 11379-11387.	3.0	48
138	Lattice dynamics of GaN/AlN superlattices. Journal of Applied Physics, 1997, 82, 622-627.	2.5	14
139	Zone-center optical phonons in wurtzite GaN and AlN. Journal of Applied Physics, 1997, 82, 4693-4695.	2.5	26
140	Lattice dynamics of zinc-blende GaN and AlN: I. Bulk phonons. Journal of Physics Condensed Matter, 1996, 8, 6323-6328.	1.8	42
141	Lattice dynamics of zinc-blende GaN and AlN: II. Superlattice phonons. Journal of Physics Condensed Matter, 1996, 8, 6329-6336.	1.8	10