

Ruhong Zhou

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/1736676/publications.pdf>

Version: 2024-02-01

321
papers

23,154
citations

9234

74
h-index

10127

140
g-index

338
all docs

338
docs citations

338
times ranked

24207
citing authors

#	ARTICLE	IF	CITATIONS
1	Graphene oxide toxicity in W1118 flies. <i>Science of the Total Environment</i> , 2022, 805, 150302.	3.9	18
2	De Novo Design of a Pt Nanocatalyst on a Conjugated Microporous Polymer-Coated Honeycomb Carrier for Oxidation of Hydrogen Isotopes. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 7826-7835.	4.0	6
3	Two-Dimensional Imprinting Strategy to Create Specific Nanotrap for Selective Uranium Adsorption with Ultrahigh Capacity. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 9408-9417.	4.0	28
4	Single nucleobase identification for transversally-confined ssDNA using longitudinal ionic currents. <i>Nanoscale</i> , 2022, , .	2.8	0
5	Role of polyplex charge density in lipopolyplex. <i>Nanoscale</i> , 2022, 14, 7174-7180.	2.8	0
6	Distinct lipid membrane interaction and uptake of differentially charged nanoplastics in bacteria. <i>Journal of Nanobiotechnology</i> , 2022, 20, 191.	4.2	30
7	Binding Affinity Calculations of Gluten Peptides to HLA Risk Modifiers: DQ2.5 versus DQ7.5. <i>Journal of Physical Chemistry B</i> , 2022, 126, 5151-5160.	1.2	2
8	Ionic Liquid Decelerates Single-Stranded DNA Transport through Molybdenum Disulfide Nanopores. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 32618-32624.	4.0	3
9	Possible Co-Evolution of Polyglutamine and Polyproline in Huntingtin Protein: Proline-Rich Domain as Transient Folding Chaperone. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 6331-6341.	2.1	3
10	Metalloï¿½Helicoid with Double Rims: Polymerization Followed by Folding by Intramolecular Coordination. <i>Angewandte Chemie</i> , 2021, 133, 1301-1309.	1.6	2
11	Metalloï¿½Helicoid with Double Rims: Polymerization Followed by Folding by Intramolecular Coordination. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 1281-1289.	7.2	18
12	Dioxybenzone triggers enhanced estrogenic effect via metabolic activation: in silico, in vitro and in vivo investigation. <i>Environmental Pollution</i> , 2021, 268, 115766.	3.7	6
13	Molecular mechanism of secreted amyloid-ï¿½ precursor protein in binding and modulating GABA _B R1a. <i>Chemical Science</i> , 2021, 12, 6107-6116.	3.7	9
14	Self-cascade MoS ₂ nanozymes for efficient intracellular antioxidation and hepatic fibrosis therapy. <i>Nanoscale</i> , 2021, 13, 12613-12622.	2.8	31
15	Molecular Dynamics Simulation Study on Interactions of Cycloviolacin with Different Phospholipids. <i>Journal of Physical Chemistry B</i> , 2021, 125, 3476-3485.	1.2	8
16	Biotransformation of rare earth oxide nanoparticles eliciting microbiota imbalance. <i>Particle and Fibre Toxicology</i> , 2021, 18, 17.	2.8	14
17	Dose-independent Transfection of Hydrophobized Polyplexes. <i>Advanced Materials</i> , 2021, 33, e2102219.	11.1	23
18	Multifaceted Regulation of Potassium-Ion Channels by Graphene Quantum Dots. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 27784-27795.	4.0	4

#	ARTICLE	IF	CITATIONS
19	CASTELO: clustered atom subtypes aided lead optimization—a combined machine learning and molecular modeling method. BMC Bioinformatics, 2021, 22, 338.	1.2	4
20	Ionic conductance oscillations in sub-nanometer pores probed by optoelectronic control. Matter, 2021, 4, 2378-2391.	5.0	13
21	Exploring an In-Plane Graphene and Hexagonal Boron Nitride Array for Separation of Single Nucleotides. ACS Nano, 2021, 15, 11704-11710.	7.3	12
22	Boron nitride nanosheets elicit significant hemolytic activity via destruction of red blood cell membranes. Colloids and Surfaces B: Biointerfaces, 2021, 203, 111765.	2.5	16
23	Hydrophobic collapse-driven nanoparticle coating with poly-adenine adhesives. Chemical Communications, 2021, 57, 3801-3804.	2.2	18
24	Modeling Noncanonical RNA Base Pairs by a Coarse-Grained IsRNA2 Model. Journal of Physical Chemistry B, 2021, 125, 11907-11915.	1.2	13
25	Molecular Insight into AC Electric Field Enhanced Removal of Protein Aggregates from a Material Surface. Journal of Physical Chemistry B, 2021, 125, 12147-12153.	1.2	0
26	Potential interference of graphene nanosheets in immune response <i>via</i> disrupting the recognition of HLA-presented KK10 by TCR: a molecular dynamics simulation study. Nanoscale, 2021, 13, 19255-19263.	2.8	4
27	Planar Boronic Graphene and Nitrogenized Graphene Heterostructure for Protein Stretch and Confinement. Biomolecules, 2021, 11, 1756.	1.8	1
28	Dynamics-Based Peptide-MHC Binding Optimization by a Convolutional Variational Autoencoder: A Use-Case Model for CASTELO. Journal of Chemical Theory and Computation, 2021, 17, 7962-7971.	2.3	7
29	HIV-1 induced changes in HLA-C α 3-presented peptide repertoires lead to reduced engagement of inhibitory natural killer cell receptors. Aids, 2020, 34, 1713-1723.	1.0	28
30	Spontaneous Translocation of Single-Stranded DNA in Graphene-MoS ₂ Heterostructure Nanopores: Shape Effect. Journal of Physical Chemistry B, 2020, 124, 9490-9496.	1.2	12
31	⁹⁹ TcO ₄ [−] removal from legacy defense nuclear waste by an alkaline-stable 2D cationic metal organic framework. Nature Communications, 2020, 11, 5571.	5.8	124
32	Low-Dose X-ray-Responsive Diselenide Nanocarriers for Effective Delivery of Anticancer Agents. ACS Applied Materials & Interfaces, 2020, 12, 43398-43407.	4.0	27
33	Partial Denaturation of Villin Headpiece upon Binding to a Carbon Nitride Polyaniline (C ₃ N) Nanosheet. Journal of Physical Chemistry B, 2020, 124, 7557-7563.	1.2	8
34	Emergence of a Radical-Stabilizing Metal-Organic Framework as a Radio-photoluminescence Dosimeter. Angewandte Chemie - International Edition, 2020, 59, 15209-15214.	7.2	56
35	Theoretical modeling of interactions at the bio-nano interface. Nanoscale, 2020, 12, 10426-10429.	2.8	7
36	Structural Basis of the Potential Binding Mechanism of Remdesivir to SARS-CoV-2 RNA-Dependent RNA Polymerase. Journal of Physical Chemistry B, 2020, 124, 6955-6962.	1.2	105

#	ARTICLE	IF	CITATIONS
37	Planar graphene/h-BN/graphene heterostructures for protein stretching and confinement. <i>Nanoscale</i> , 2020, 12, 13822-13828.	2.8	15
38	Tungsten Oxide Nanodots Exhibit Mild Interactions with WW and SH3 Modular Protein Domains. <i>ACS Omega</i> , 2020, 5, 11005-11012.	1.6	1
39	A Porous Aromatic Framework Functionalized with Luminescent Iridium(III) Organometallic Complexes for Turn-On Sensing of $^{99}\text{TcO}_4^-$. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 15288-15297.	4.0	46
40	In silico design and validation of high-affinity RNA aptamers targeting epithelial cellular adhesion molecule dimers. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 8486-8493.	3.3	49
41	Graphene-extracted membrane lipids facilitate the activation of integrin $\alpha_5\beta_1$. <i>Nanoscale</i> , 2020, 12, 7939-7949.	2.8	22
42	Half a century of amyloids: past, present and future. <i>Chemical Society Reviews</i> , 2020, 49, 5473-5509.	18.7	345
43	Stabilization of Open-Shell Single Bonds within Endohedral Metallofullerene. <i>Inorganic Chemistry</i> , 2020, 59, 3606-3618.	1.9	11
44	Directional extraction and penetration of phosphorene nanosheets to cell membranes. <i>Nanoscale</i> , 2020, 12, 2810-2819.	2.8	27
45	Retained Stability of the RNA Structure in DNA Packaging Motor with a Single Mg^{2+} Ion Bound at the Double Mg-Clamp Structure. <i>Journal of Physical Chemistry B</i> , 2020, 124, 701-707.	1.2	4
46	<i>N</i> -Oxide polymer-cupric ion nanogels potentiate disulfiram for cancer therapy. <i>Biomaterials Science</i> , 2020, 8, 1726-1733.	2.6	11
47	Zipper-Like Unfolding of dsDNA Caused by Graphene Wrinkles. <i>Journal of Physical Chemistry C</i> , 2020, 124, 3332-3340.	1.5	11
48	Electron Beam Irradiation as a General Approach for the Rapid Synthesis of Covalent Organic Frameworks under Ambient Conditions. <i>Journal of the American Chemical Society</i> , 2020, 142, 9169-9174.	6.6	90
49	Binding patterns and dynamics of double-stranded DNA on the phosphorene surface. <i>Nanoscale</i> , 2020, 12, 9430-9439.	2.8	17
50	Emergence of a Radical-Stabilizing Metal-Organic Framework as a Radio-photoluminescence Dosimeter. <i>Angewandte Chemie</i> , 2020, 132, 15321-15326.	1.6	14
51	Proteasome activity regulated by charged gold nanoclusters: Implications for neurodegenerative diseases. <i>Nano Today</i> , 2020, 35, 100933.	6.2	10
52	Commensal bacteria stimulate antitumor responses via T cell cross-reactivity. <i>JCI Insight</i> , 2020, 5, .	2.3	95
53	Exploration of HIV-1 fusion peptide-antibody VRC34.01 binding reveals fundamental neutralization sites. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 18569-18576.	1.3	5
54	Lanosterol Disrupts the Aggregation of Amyloid- β Peptides. <i>ACS Chemical Neuroscience</i> , 2019, 10, 4051-4060.	1.7	14

#	ARTICLE	IF	CITATIONS
55	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
56	Stability of Ligands on Nanoparticles Regulating the Integrity of Biological Membranes at the Nano-Lipid Interface. <i>ACS Nano</i> , 2019, 13, 8680-8693.	7.3	59
57	Surface Inhomogeneity of Graphene Oxide Influences Dissociation of $\text{A}\beta_{21}$ Peptide Assembly. <i>Journal of Physical Chemistry B</i> , 2019, 123, 9098-9103.	1.2	13
58	Spontaneous ssDNA stretching on graphene and hexagonal boron nitride in plane heterostructures. <i>Nature Communications</i> , 2019, 10, 4610.	5.8	36
59	Stimulating antibacterial activities of graphitic carbon nitride nanosheets with plasma treatment. <i>Nanoscale</i> , 2019, 11, 18416-18425.	2.8	41
60	Different platinum crystal surfaces show very distinct protein denaturation capabilities. <i>Nanoscale</i> , 2019, 11, 19352-19361.	2.8	3
61	Modeling and Structural Characterization of the Sweet Taste Receptor Heterodimer. <i>ACS Chemical Neuroscience</i> , 2019, 10, 4579-4592.	1.7	18
62	Facet-regulated adhesion of double-stranded DNA on palladium surfaces. <i>Nanoscale</i> , 2019, 11, 1827-1836.	2.8	11
63	Inorganic X-ray Scintillators Based on a Previously Unnoticed but Intrinsically Advantageous Metal Center. <i>Inorganic Chemistry</i> , 2019, 58, 2807-2812.	1.9	13
64	Robust Antibacterial Activity of Tungsten Oxide (WO_3) Nanodots. <i>Chemical Research in Toxicology</i> , 2019, 32, 1357-1366.	1.7	73
65	A 3,2-Hydroxypyridinone-based Decorporation Agent that Removes Uranium from Bones In Vivo. <i>Nature Communications</i> , 2019, 10, 2570.	5.8	107
66	A Public BCR Present in a Unique Dual-Receptor-Expressing Lymphocyte from Type 1 Diabetes Patients Encodes a Potent T Cell Autoantigen. <i>Cell</i> , 2019, 177, 1583-1599.e16.	13.5	103
67	Different protonated states at the C-terminal of the amyloid- β_2 peptide modulate the stability of S-shaped protofibril. <i>Journal of Chemical Physics</i> , 2019, 150, 185102.	1.2	3
68	Molecular Origin of the Stability Difference in Four Shark IgNAR Constant Domains. <i>Biophysical Journal</i> , 2019, 116, 1907-1917.	0.2	6
69	Defect-assisted protein HP35 denaturation on graphene. <i>Nanoscale</i> , 2019, 11, 19362-19369.	2.8	30
70	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
71	Protein WW domain denaturation on defective graphene reveals the significance of nanomaterial defects in nanotoxicity. <i>Carbon</i> , 2019, 146, 257-264.	5.4	24
72	Mechanism unravelling for ultrafast and selective $^{99}\text{TcO}_4^-$ uptake by a radiation-resistant cationic covalent organic framework: a combined radiological experiment and molecular dynamics simulation study. <i>Chemical Science</i> , 2019, 10, 4293-4305.	3.7	181

#	ARTICLE	IF	CITATIONS
73	Successful Decontamination of $^{99}\text{TcO}_4^-$ in Groundwater at Legacy Nuclear Sites by a Cationic Metal-Organic Framework with Hydrophobic Pockets. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 4968-4972.	7.2	177
74	Successful Decontamination of $^{99}\text{TcO}_4^-$ in Groundwater at Legacy Nuclear Sites by a Cationic Metal-Organic Framework with Hydrophobic Pockets. <i>Angewandte Chemie</i> , 2019, 131, 5022-5026.	1.6	37
75	The molecular mechanism of robust macrophage immune responses induced by PEGylated molybdenum disulfide. <i>Nanoscale</i> , 2019, 11, 22293-22304.	2.8	35
76	Physical and toxicological profiles of human IAPP amyloids and plaques. <i>Science Bulletin</i> , 2019, 64, 26-35.	4.3	24
77	Atomic-Scale Fluidic Diodes Based on Triangular Nanopores in Bilayer Hexagonal Boron Nitride. <i>Nano Letters</i> , 2019, 19, 977-982.	4.5	31
78	Exploring the binding mechanism between human profilin (PFN1) and polyproline-10 through binding mode screening. <i>Journal of Chemical Physics</i> , 2019, 150, 015102.	1.2	4
79	Charging nanoparticles: increased binding of $\text{Gd}@C_{82}(\text{OH})_{22}$ derivatives to human MMP-9. <i>Nanoscale</i> , 2018, 10, 5667-5677.	2.8	25
80	$\text{C}=\text{O}^-$ K^+ (Na^+) groups in non-doped carbon as active sites for the oxygen reduction reaction. <i>Journal of Materials Chemistry A</i> , 2018, 6, 8955-8961.	5.2	28
81	Unique Proton Transportation Pathway in a Robust Inorganic Coordination Polymer Leading to Intrinsically High and Sustainable Anhydrous Proton Conductivity. <i>Journal of the American Chemical Society</i> , 2018, 140, 6146-6155.	6.6	181
82	Rare Dissipative Transitions Punctuate the Initiation of Chemical Denaturation in Proteins. <i>Biophysical Journal</i> , 2018, 114, 812-821.	0.2	0
83	Spontaneous Transport of Single-Stranded DNA through Graphene-MoS ₂ Heterostructure Nanopores. <i>ACS Nano</i> , 2018, 12, 3886-3891.	7.3	57
84	Facile and Efficient Decontamination of Thorium from Rare Earths Based on Selective Selenite Crystallization. <i>Inorganic Chemistry</i> , 2018, 57, 1880-1887.	1.9	32
85	Inhibition of the proteasome activity by graphene oxide contributes to its cytotoxicity. <i>Nanotoxicology</i> , 2018, 12, 185-200.	1.6	14
86	T cell receptors for the HIV KK10 epitope from patients with differential immunologic control are functionally indistinguishable. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 1877-1882.	3.3	15
87	Inhibition of CYP2C8 by metallofullerenol $\text{Gd}@C_{82}(\text{OH})_{22}$ through blocking substrate channels and substrate recognition sites. <i>Carbon</i> , 2018, 127, 667-675.	5.4	9
88	Phase transition triggered aggregation-induced emission in a photoluminescent uranyl-organic framework. <i>Chemical Communications</i> , 2018, 54, 627-630.	2.2	35
89	Binding Specificity Determines the Cytochrome P450 3A4 Mediated Enantioselective Metabolism of Metconazole. <i>Journal of Physical Chemistry B</i> , 2018, 122, 1176-1184.	1.2	29
90	Highly Sensitive Detection of UV Radiation Using a Uranium Coordination Polymer. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 4844-4850.	4.0	52

#	ARTICLE	IF	CITATIONS
91	Differential Pd-nanocrystal facets demonstrate distinct antibacterial activity against Gram-positive and Gram-negative bacteria. <i>Nature Communications</i> , 2018, 9, 129.	5.8	414
92	An Ultrastable Heterobimetallic Uranium(IV)/Vanadium(III) Solid Compound Protected by a Redox-Active Phosphite Ligand: Crystal Structure, Oxidative Dissolution, and First-Principles Simulation. <i>Inorganic Chemistry</i> , 2018, 57, 903-907.	1.9	8
93	Mechanism by which DHA inhibits the aggregation of KLVFFA peptides: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 2018, 148, 115102.	1.2	7
94	Molecular mechanism of Gd@C 82 (OH) 22 increasing collagen expression: Implication for encaging tumor. <i>Biomaterials</i> , 2018, 152, 24-36.	5.7	26
95	Exploring the Nanotoxicology of MoS ₂ : A Study on the Interaction of MoS ₂ Nanoflakes and K ⁺ Channels. <i>ACS Nano</i> , 2018, 12, 705-717.	7.3	44
96	Patient HLA class I genotype influences cancer response to checkpoint blockade immunotherapy. <i>Science</i> , 2018, 359, 582-587.	6.0	834
97	Concentration-dependent binding of CdSe quantum dots on the SH3 domain. <i>Nanoscale</i> , 2018, 10, 351-358.	2.8	8
98	Metal-organic framework as an efficient filter for the removal of heavy metal cations in water. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 30384-30391.	1.3	20
99	Palladium concave nanocrystals with high-index facets accelerate ascorbate oxidation in cancer treatment. <i>Nature Communications</i> , 2018, 9, 4861.	5.8	84
100	Superior Compatibility of C ₂ N with Human Red Blood Cell Membranes and the Underlying Mechanism. <i>Small</i> , 2018, 14, e1803509.	5.2	33
101	Molecular mechanism of phosphoinositides' specificity for the inwardly rectifying potassium channel Kir2.2. <i>Chemical Science</i> , 2018, 9, 8352-8362.	3.7	2
102	Degradable Carbon Dots with Broad-Spectrum Antibacterial Activity. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 26936-26946.	4.0	246
103	Glassy dynamics in mutant huntingtin proteins. <i>Journal of Chemical Physics</i> , 2018, 149, 072333.	1.2	9
104	Single-File Protein Translocations through Graphene-MoS ₂ Heterostructure Nanopores. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3409-3415.	2.1	45
105	Lanosterol Disrupts Aggregation of Human ³ D-Crystallin by Binding to the Hydrophobic Dimerization Interface. <i>Journal of the American Chemical Society</i> , 2018, 140, 8479-8486.	6.6	42
106	Membrane Insertion and Phospholipids Extraction by Graphyne Nanosheets. <i>Journal of Physical Chemistry C</i> , 2017, 121, 2444-2450.	1.5	31
107	High-Curvature Nanostructuring Enhances Probe Display for Biomolecular Detection. <i>Nano Letters</i> , 2017, 17, 1289-1295.	4.5	64
108	Mild Binding of Protein to C ₂ N Monolayer Reveals Its Suitable Biocompatibility. <i>Small</i> , 2017, 13, 1603685.	5.2	37

#	ARTICLE	IF	CITATIONS
109	Graphene-Induced Pore Formation on Cell Membranes. <i>Scientific Reports</i> , 2017, 7, 42767.	1.6	103
110	Highly Sensitive and Selective Uranium Detection in Natural Water Systems Using a Luminescent Mesoporous Metal-Organic Framework Equipped with Abundant Lewis Basic Sites: A Combined Batch, X-ray Absorption Spectroscopy, and First Principles Simulation Investigation. <i>Environmental Science & Technology</i> , 2017, 51, 3911-3921.	4.6	331
111	PEGylated graphene oxide elicits strong immunological responses despite surface passivation. <i>Nature Communications</i> , 2017, 8, 14537.	5.8	157
112	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
113	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
114	Exceptional Perrhenate/Pertechnetate Uptake and Subsequent Immobilization by a Low-Dimensional Cationic Coordination Polymer: Overcoming the Hofmeister Bias Selectivity. <i>Environmental Science and Technology Letters</i> , 2017, 4, 316-322.	3.9	181
115	Overcoming the crystallization and designability issues in the ultrastable zirconium phosphonate framework system. <i>Nature Communications</i> , 2017, 8, 15369.	5.8	366
116	Understanding the graphene quantum dots-ubiquitin interaction by identifying the interaction sites. <i>Carbon</i> , 2017, 121, 285-291.	5.4	17
117	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
118	Impact of graphyne on structural and dynamical properties of calmodulin. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 10187-10195.	1.3	10
119	Orientational Binding of DNA Guided by the C_{2v} N Template. <i>ACS Nano</i> , 2017, 11, 3198-3206.	7.3	51
120	Structural influence of proteins upon adsorption to MoS_2 nanomaterials: comparison of MoS_2 force field parameters. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 3039-3045.	1.3	43
121	Snatching the Ligand or Destroying the Structure: Disruption of WW Domain by Phosphorene. <i>Journal of Physical Chemistry C</i> , 2017, 121, 1362-1370.	1.5	14
122	Identifying the Recognition Site for Selective Trapping of $^{99}TcO_4^-$ in a Hydrolytically Stable and Radiation Resistant Cationic Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2017, 139, 14873-14876.	6.6	386
123	Hydrogen and methane storage and release by MoS_2 nanotubes for energy storage. <i>Journal of Materials Chemistry A</i> , 2017, 5, 23020-23027.	5.2	33
124	Phosphatidylserine-Induced Conformational Modulation of Immune Cell Exhaustion-Associated Receptor TIM3. <i>Scientific Reports</i> , 2017, 7, 13579.	1.6	8
125	Directional mechanical stability of Bacteriophage ϕ 29 motor's 3WJ-pRNA: Extraordinary robustness along portal axis. <i>Science Advances</i> , 2017, 3, e1601684.	4.7	17
126	Hydroxyl-Group-Dominated Graphite Dots Reshape Laser Desorption/Ionization Mass Spectrometry for Small Biomolecular Analysis and Imaging. <i>ACS Nano</i> , 2017, 11, 9500-9513.	7.3	79

#	ARTICLE	IF	CITATIONS
127	Humidity-Responsive Single-Nanoparticle-Layer Plasmonic Films. <i>Advanced Materials</i> , 2017, 29, 1606796.	11.1	25
128	Thickness dependent semiconductor-to-metal transition of two-dimensional polyaniline with unique work functions. <i>Nanoscale</i> , 2017, 9, 12025-12031.	2.8	24
129	Structural perturbations on huntingtin N17 domain during its folding on 2D-nanomaterials. <i>Nanotechnology</i> , 2017, 28, 354001.	1.3	12
130	Membrane destruction-mediated antibacterial activity of tungsten disulfide (WS ₂). <i>RSC Advances</i> , 2017, 7, 37873-37880.	1.7	76
131	Detecting Interactions between Nanomaterials and Cell Membranes by Synthetic Nanopores. <i>ACS Nano</i> , 2017, 11, 12615-12623.	7.3	25
132	A mesoporous cationic thorium-organic framework that rapidly traps anionic persistent organic pollutants. <i>Nature Communications</i> , 2017, 8, 1354.	5.8	296
133	Graphene Oxide Nanosheets Retard Cellular Migration via Disruption of Actin Cytoskeleton. <i>Small</i> , 2017, 13, 1602133.	5.2	68
134	Propensity of a single-walled carbon nanotube-peptide to mimic a KK10 peptide in an HLA-TCR complex. <i>Journal of Chemical Physics</i> , 2017, 147, 225101.	1.2	3
135	A new molecular mechanism underlying the EGCG-mediated autophagic modulation of AFP in HepG2 cells. <i>Cell Death and Disease</i> , 2017, 8, e3160-e3160.	2.7	48
136	An In Silico study of TiO ₂ nanoparticles interaction with twenty standard amino acids in aqueous solution. <i>Scientific Reports</i> , 2016, 6, 37761.	1.6	40
137	EGCG in Green Tea Induces Aggregation of HMGB1 Protein through Large Conformational Changes with Polarized Charge Redistribution. <i>Scientific Reports</i> , 2016, 6, 22128.	1.6	19
138	Molecular Structure and Dynamics of Water on Pristine and Strained Phosphorene: Wetting and Diffusion at Nanoscale. <i>Scientific Reports</i> , 2016, 6, 38327.	1.6	30
139	Potential disruption of protein-protein interactions by graphene oxide. <i>Journal of Chemical Physics</i> , 2016, 144, 225102.	1.2	24
140	Exploring biological effects of MoS ₂ nanosheets on native structures of α -helical peptides. <i>Journal of Chemical Physics</i> , 2016, 144, 175103.	1.2	37
141	Wettability and friction of water on a MoS ₂ nanosheet. <i>Applied Physics Letters</i> , 2016, 108, .	1.5	113
142	Structural Damage of a β -Sheet Protein upon Adsorption onto Molybdenum Disulfide Nanotubes. <i>Journal of Physical Chemistry C</i> , 2016, 120, 6796-6803.	1.5	39
143	Polymeric prodrugs conjugated with reduction-sensitive dextran-camptothecin and pH-responsive dextran-doxorubicin: an effective combinatorial drug delivery platform for cancer therapy. <i>Polymer Chemistry</i> , 2016, 7, 4198-4212.	1.9	53
144	Self-Assembled Core-Satellite Gold Nanoparticle Networks for Ultrasensitive Detection of Chiral Molecules by Recognition Tunneling Current. <i>ACS Nano</i> , 2016, 10, 5096-5103.	7.3	47

#	ARTICLE	IF	CITATIONS
145	The Molecular Mechanism of Opening the Helix Bundle Crossing (HBC) Gate of a Kir Channel. <i>Scientific Reports</i> , 2016, 6, 29399.	1.6	26
146	Robust Denaturation of Villin Headpiece by MoS ₂ Nanosheet: Potential Molecular Origin of the Nanotoxicity. <i>Scientific Reports</i> , 2016, 6, 28252.	1.6	33
147	Single-Walled Carbon Nanotubes Inhibit the Cytochrome P450 Enzyme, CYP3A4. <i>Scientific Reports</i> , 2016, 6, 21316.	1.6	43
148	Folding and Stabilization of Native-Sequence-Reversed Proteins. <i>Scientific Reports</i> , 2016, 6, 25138.	1.6	6
149	Mechanism of Divalent-Ion-Induced Charge Inversion of Bacterial Membranes. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2434-2438.	2.1	20
150	Exploring the Membrane Potential of Simple Dual-Membrane Systems as Models for Gap-Junction Channels. <i>Biophysical Journal</i> , 2016, 110, 2678-2688.	0.2	14
151	Opening Lids: Modulation of Lipase Immobilization by Graphene Oxides. <i>ACS Catalysis</i> , 2016, 6, 4760-4768.	5.5	139
152	Tunable, Strain-Controlled Nanoporous MoS ₂ Filter for Water Desalination. <i>ACS Nano</i> , 2016, 10, 1829-1835.	7.3	212
153	Sequential protein unfolding through a carbon nanotube pore. <i>Nanoscale</i> , 2016, 8, 12143-12151.	2.8	17
154	Complete wetting of graphene by biological lipids. <i>Nanoscale</i> , 2016, 8, 5750-5754.	2.8	83
155	Potential Interference of Protein-Protein Interactions by Graphyne. <i>Journal of Physical Chemistry B</i> , 2016, 120, 2124-2131.	1.2	18
156	Toward high permeability, selectivity and controllability of water desalination with FePc nanopores. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 8140-8147.	1.3	11
157	Nanomechanics of Protein Unfolding Outside a Generic Nanopore. <i>ACS Nano</i> , 2016, 10, 317-323.	7.3	27
158	DNA translocation through single-layer boron nitride nanopores. <i>Soft Matter</i> , 2016, 12, 817-823.	1.2	49
159	Selection of an HLA-C*03:04-Restricted HIV-1 p24 Gag Sequence Variant Is Associated with Viral Escape from KIR2DL3+ Natural Killer Cells: Data from an Observational Cohort in South Africa. <i>PLoS Medicine</i> , 2015, 12, e1001900.	3.9	66
160	Reduced Cytotoxicity of Graphene Nanosheets Mediated by Blood-Protein Coating. <i>ACS Nano</i> , 2015, 9, 5713-5724.	7.3	271
161	Bio-mimicking of Proline-Rich Motif Applied to Carbon Nanotube Reveals Unexpected Subtleties Underlying Nanoparticle Functionalization. <i>Scientific Reports</i> , 2015, 4, 7229.	1.6	4
162	Ionic liquid induced inactivation of cellobiohydrolase I from <i>Trichoderma reesei</i> . <i>Green Chemistry</i> , 2015, 17, 1618-1625.	4.6	22

#	ARTICLE	IF	CITATIONS
163	Hydrated Excess Protons Can Create Their Own Water Wires. <i>Journal of Physical Chemistry B</i> , 2015, 119, 9212-9218.	1.2	83
164	Towards understanding of nanoparticle-protein corona. <i>Archives of Toxicology</i> , 2015, 89, 519-539.	1.9	135
165	Nanopore-Based Sensors for Ligand-Receptor Lead Optimization. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 331-337.	2.1	5
166	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
167	Even with nonnative interactions, the updated folding transition states of the homologs Proteins G & L are extensive and similar. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 8302-8307.	3.3	21
168	Gd-Metallofullerenol Nanomaterial Suppresses Pancreatic Cancer Metastasis by Inhibiting the Interaction of Histone Deacetylase 1 and Metastasis-Associated Protein 1. <i>ACS Nano</i> , 2015, 9, 6826-6836.	7.3	64
169	Simplified TiO ₂ force fields for studies of its interaction with biomolecules. <i>Journal of Chemical Physics</i> , 2015, 142, 234102.	1.2	41
170	A Peptide-Coated Gold Nanocluster Exhibits Unique Behavior in Protein Activity Inhibition. <i>Journal of the American Chemical Society</i> , 2015, 137, 8412-8418.	6.6	79
171	Surface Curvature Relation to Protein Adsorption for Carbon-based Nanomaterials. <i>Scientific Reports</i> , 2015, 5, 10886.	1.6	97
172	The role of basic residues in the adsorption of blood proteins onto the graphene surface. <i>Scientific Reports</i> , 2015, 5, 10873.	1.6	88
173	Water film inside graphene nanosheets: electron transfer reversal between water and graphene via tight nano-confinement. <i>RSC Advances</i> , 2015, 5, 274-280.	1.7	17
174	Quantum Dots and Their Ligand Passivation. , 2015, , 131-145.		0
175	Exploration of graphene oxide as an intelligent platform for cancer vaccines. <i>Nanoscale</i> , 2015, 7, 19949-19957.	2.8	49
176	Destruction of amyloid fibrils by graphene through penetration and extraction of peptides. <i>Nanoscale</i> , 2015, 7, 18725-18737.	2.8	101
177	Nanomedicine: Implications from Nanotoxicity. , 2015, , 147-168.		0
178	Fullerene and Derivatives. , 2015, , 17-43.		0
179	Protein corona mitigates the cytotoxicity of graphene oxide by reducing its physical interaction with cell membrane. <i>Nanoscale</i> , 2015, 7, 15214-15224.	2.8	204
180	A novel form of β -strand assembly observed in Au^{3+} adsorbed onto graphene. <i>Nanoscale</i> , 2015, 7, 15341-15348.	2.8	23

#	ARTICLE	IF	CITATIONS
181	Potential Toxicity of Graphene to Cell Functions via Disrupting Protein-Protein Interactions. ACS Nano, 2015, 9, 663-669.	7.3	164
182	Structural and electronic properties of uranium-encapsulated Au ₁₄ cage. Scientific Reports, 2015, 4, 5862.	1.6	29
183	Graphyne and Derivatives. , 2015, , 89-100.		0
184	Noble Metal Nanomaterials. , 2015, , 101-113.		0
185	Metal Oxides and Related Nanostructures. , 2015, , 115-130.		1
186	Dewetting transition assisted clearance of (NFGAILS) amyloid fibrils from cell membranes by graphene. Journal of Chemical Physics, 2014, 141, 22D520.	1.2	16
187	The ground state and electronic structure of Gd@C82: A systematic theoretical investigation of first principle density functionals. Journal of Chemical Physics, 2014, 141, 244306.	1.2	22
188	A unique feature of chiral transition of a difluorobenzo[c]phenanthrene molecule confined in a boron-nitride nanotube based on molecular dynamics simulations. Chemical Physics Letters, 2014, 591, 265-267.	1.2	5
189	How force unfolding differs from chemical denaturation. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 3413-3418.	3.3	83
190	Conformation-dependent DNA attraction. Nanoscale, 2014, 6, 7085-7092.	2.8	13
191	Molecular Recognition of Metabotropic Glutamate Receptor Type 1 (mGluR1): Synergistic Understanding with Free Energy Perturbation and Linear Response Modeling. Journal of Physical Chemistry B, 2014, 118, 6393-6404.	1.2	2
192	Nanomedicine: de novo design of nanodrugs. Nanoscale, 2014, 6, 663-677.	2.8	56
193	Irreversible Denaturation of Proteins through Aluminum-Induced Formation of Backbone Ring Structures. Angewandte Chemie - International Edition, 2014, 53, 6358-6363.	7.2	20
194	Effect of ligands on the characteristics of (CdSe) ₁₃ quantum dots. RSC Advances, 2014, 4, 27146-27151.	1.7	23
195	Dissecting the contributions of ¹² I-hairpin tyrosine pairs to the folding and stability of long-lived human ¹³ D-crystallins. Nanoscale, 2014, 6, 1797-1807.	2.8	11
196	Cytotoxicity of graphene: recent advances and future perspective. Wiley Interdisciplinary Reviews: Nanomedicine and Nanobiotechnology, 2014, 6, 452-474.	3.3	101
197	Effect of Urea Concentration on Aggregation of Amyloidogenic Hexapeptides (NFGAIL). Journal of Physical Chemistry B, 2014, 118, 48-57.	1.2	14
198	Characterization of a Novel Water Pocket Inside the Human Cx26 Hemichannel Structure. Biophysical Journal, 2014, 107, 599-612.	0.2	34

#	ARTICLE	IF	CITATIONS
199	An improved DNA force field for ssDNA interactions with gold nanoparticles. <i>Journal of Chemical Physics</i> , 2014, 140, 234102.	1.2	12
200	Controlled transport of DNA through a Y-shaped carbon nanotube in a solid membrane. <i>Nanoscale</i> , 2014, 6, 11479-11483.	2.8	11
201	Carbon nanotubes adsorb U atoms differently in their inner and outer surfaces. <i>RSC Advances</i> , 2014, 4, 30074.	1.7	10
202	Path Integral Coarse-Graining Replica Exchange Method for Enhanced Sampling. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3634-3640.	2.3	11
203	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.	2.8	100
204	Size-dependent impact of CNTs on dynamic properties of calmodulin. <i>Nanoscale</i> , 2014, 6, 12828-12837.	2.8	18
205	Large scale molecular simulations of nanotoxicity. <i>Wiley Interdisciplinary Reviews: Systems Biology and Medicine</i> , 2014, 6, 329-343.	6.6	34
206	The complex and specific pMHC interactions with diverse HIV-1 TCR clonotypes reveal a structural basis for alterations in CTL function. <i>Scientific Reports</i> , 2014, 4, 4087.	1.6	22
207	Dual Inhibitory Pathways of Metallofullerenol Gd@C82(OH)22 on Matrix Metalloproteinase-2: Molecular insight into drug-like nanomedicine. <i>Scientific Reports</i> , 2014, 4, 4775.	1.6	25
208	Rotation Motion of Designed Nano-Turbine. <i>Scientific Reports</i> , 2014, 4, 5846.	1.6	27
209	Binding Preference of Carbon Nanotube Over Proline-Rich Motif Ligand on SH3-Domain: A Comparison with Different Force Fields. <i>Journal of Physical Chemistry B</i> , 2013, 117, 3541-3547.	1.2	14
210	The ice-like water monolayer near the wall makes inner water shells diffuse faster inside a charged nanotube. <i>Journal of Chemical Physics</i> , 2013, 138, 204710.	1.2	18
211	Interactions Between Proteins and Carbon-Based Nanoparticles: Exploring the Origin of Nanotoxicity at the Molecular Level. <i>Small</i> , 2013, 9, 1546-1556.	5.2	132
212	Capability of charge signal conversion and transmission by water chains confined inside Y-shaped carbon nanotubes. <i>Journal of Chemical Physics</i> , 2013, 138, 015104.	1.2	11
213	Metallofullerenol Gd@C82(OH)22 distracts the proline-rich-motif from putative binding on the SH3 domain. <i>Nanoscale</i> , 2013, 5, 2703.	2.8	22
214	Ethanol promotes dewetting transition at low concentrations. <i>Soft Matter</i> , 2013, 9, 4655.	1.2	20
215	Hydrophobic Interaction Drives Surface-Assisted Epitaxial Assembly of Amyloid-like Peptides. <i>Journal of the American Chemical Society</i> , 2013, 135, 3150-3157.	6.6	56
216	Impacts of fullerene derivatives on regulating the structure and assembly of collagen molecules. <i>Nanoscale</i> , 2013, 5, 7341.	2.8	24

#	ARTICLE	IF	CITATIONS
217	Destructive extraction of phospholipids from Escherichia coli membranes by graphene nanosheets. Nature Nanotechnology, 2013, 8, 594-601.	15.6	1,260
218	Interplay between Drying and Stability of a TIM Barrel Protein: A Combined Simulation"Experimental Study. Journal of the American Chemical Society, 2013, 135, 1882-1890.	6.6	22
219	Collapse of a Hydrophobic Polymer in a Mixture of Denaturants. Langmuir, 2013, 29, 4877-4882.	1.6	18
220	Salts drive controllable multilayered upright assembly of amyloid-like peptides at mica/water interface. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 8543-8548.	3.3	46
221	UV-radiation Induced Disruption of Dry-Cavities in Human $\hat{3}$ D-crystallin Results in Decreased Stability and Faster Unfolding. Scientific Reports, 2013, 3, 1560.	1.6	37
222	Large Domain Motions in Ago Protein Controlled by the Guide DNA-Strand Seed Region Determine the Ago-DNA-mRNA Complex Recognition Process. PLoS ONE, 2013, 8, e54620.	1.1	16
223	Non-destructive Inhibition of Metallofullerenol Gd@C ₈₂ (OH) ₂₂ on WW domain: Implication on Signal Transduction Pathway. Scientific Reports, 2012, 2, 957.	1.6	41
224	Molecular mechanism of pancreatic tumor metastasis inhibition by Gd@C ₈₂ (OH) ₂₂ and its implication for de novo design of nanomedicine. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 15431-15436.	3.3	200
225	Dynamics of DNA translocation in a solid-state nanopore immersed in aqueous glycerol. Nanotechnology, 2012, 23, 455102.	1.3	33
226	Enantiomerization Mechanism of Thalidomide and the Role of Water and Hydroxide Ions. Chemistry - A European Journal, 2012, 18, 14305-14313.	1.7	30
227	Molecular wire of urea in carbon nanotube: a molecular dynamics study. Nanoscale, 2012, 4, 652-658.	2.8	20
228	Probing the Self-Assembly Mechanism of Diphenylalanine-Based Peptide Nanovesicles and Nanotubes. ACS Nano, 2012, 6, 3907-3918.	7.3	264
229	How does water-nanotube interaction influence water flow through the nanochannel?. Journal of Chemical Physics, 2012, 136, 175101.	1.2	16
230	Modelling of the nanoscale. Nanoscale, 2012, 4, 1042.	2.8	7
231	Nanopore-Based Sensors for Detecting Toxicity of a Carbon Nanotube to Proteins. Journal of Physical Chemistry Letters, 2012, 3, 2337-2341.	2.1	17
232	Molecular Mechanism of Surface-Assisted Epitaxial Self-Assembly of Amyloid-like Peptides. ACS Nano, 2012, 6, 9276-9282.	7.3	29
233	The Folding Transition State of Protein L Is Extensive with Nonnative Interactions (and Not Small and) Tj ETQq1 1 0,784314 rgBT /Ovele	2.0	28
234	Collapse of Unfolded Proteins in a Mixture of Denaturants. Journal of the American Chemical Society, 2012, 134, 18266-18274.	6.6	55

#	ARTICLE	IF	CITATIONS
235	Free-Energy Simulations Reveal that Both Hydrophobic and Polar Interactions Are Important for Influenza Hemagglutinin Antibody Binding. <i>Biophysical Journal</i> , 2012, 102, 1453-1461.	0.2	30
236	Salting Effects on Protein Components in Aqueous NaCl and Urea Solutions: Toward Understanding of Urea-Induced Protein Denaturation. <i>Journal of Physical Chemistry B</i> , 2012, 116, 1446-1451.	1.2	38
237	Novel Design of a Nanoflowmeter Based on Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2012, 116, 13429-13434.	1.5	7
238	Molecular dynamics simulations of Ago silencing complexes reveal a large repertoire of admissible "seed-less" targets. <i>Scientific Reports</i> , 2012, 2, 569.	1.6	62
239	Conformational Changes of the Protein Domains Upon Binding with Carbon Nanotubes Studied by Molecular Dynamics Simulations. <i>Current Physical Chemistry</i> , 2012, 2, 12-22.	0.1	7
240	Amino acid analogues bind to carbon nanotube via π - π interactions: Comparison of molecular mechanical and quantum mechanical calculations. <i>Journal of Chemical Physics</i> , 2012, 136, 025103.	1.2	103
241	Coherent Microscopic Picture for Urea-Induced Denaturation of Proteins. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8856-8862.	1.2	29
242	Comprehensive interrogation of natural TALE DNA-binding modules and transcriptional repressor domains. <i>Nature Communications</i> , 2012, 3, 968.	5.8	291
243	Multiscale modeling of macromolecular biosystems. <i>Briefings in Bioinformatics</i> , 2012, 13, 395-405.	3.2	29
244	Binding of blood proteins to carbon nanotubes reduces cytotoxicity. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 16968-16973.	3.3	839
245	Carbon Nanotube Wins the Competitive Binding over Proline-Rich Motif Ligand on SH3 Domain. <i>Journal of Physical Chemistry C</i> , 2011, 115, 12322-12328.	1.5	56
246	Comment on "Urea-Mediated Protein Denaturation: A Consensus View". <i>Journal of Physical Chemistry B</i> , 2011, 115, 1323-1326.	1.2	35
247	Urea-Induced Drying of Hydrophobic Nanotubes: Comparison of Different Urea Models. <i>Journal of Physical Chemistry B</i> , 2011, 115, 2988-2994.	1.2	52
248	Dewetting Transitions in the Self-Assembly of Two Amyloidogenic β -Sheets and the Importance of Matching Surfaces. <i>Journal of Physical Chemistry B</i> , 2011, 115, 11137-11144.	1.2	27
249	Aggregation of β -crystallins associated with human cataracts via domain swapping at the C-terminal β -strands. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 10514-10519.	3.3	117
250	Nanotoxicity: Exploring the Interactions Between Carbon Nanotubes and Proteins. , 2011, , .		2
251	Adsorption of Villin Headpiece onto Graphene, Carbon Nanotube, and C60: Effect of Contacting Surface Curvatures on Binding Affinity. <i>Journal of Physical Chemistry C</i> , 2011, 115, 23323-23328.	1.5	181
252	β -strand interactions at the domain interface critical for the stability of human lens β -crystallin. <i>Protein Science</i> , 2010, 19, 131-140.	3.1	38

#	ARTICLE	IF	CITATIONS
253	Size Dependence of Nanoscale Confinement on Chiral Transformation. <i>Chemistry - A European Journal</i> , 2010, 16, 6482-6487.	1.7	6
254	Plugging into Proteins: Poisoning Protein Function by a Hydrophobic Nanoparticle. <i>ACS Nano</i> , 2010, 4, 7508-7514.	7.3	168
255	Single Mutation Effects on Conformational Change and Membrane Deformation of Influenza Hemagglutinin Fusion Peptides. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8799-8806.	1.2	33
256	Key Residues that Play a Critical Role in Urea-Induced Lysozyme Unfolding. <i>Journal of Physical Chemistry B</i> , 2010, 114, 15687-15693.	1.2	19
257	Molecular Dynamics with Multiple Time Scales: How to Avoid Pitfalls. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1798-1804.	2.3	57
258	Urea-Induced Drying of Carbon Nanotubes Suggests Existence of a Dry Globule-like Transient State During Chemical Denaturation of Proteins. <i>Journal of Physical Chemistry B</i> , 2010, 114, 5427-5430.	1.2	58
259	Signal transmission, conversion and multiplication by polar molecules confined in nanochannels. <i>Nanoscale</i> , 2010, 2, 1976.	2.8	33
260	Water-mediated signal multiplication with Y-shaped carbon nanotubes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 18120-18124.	3.3	120
261	Linear interaction energy approximation for binding affinities of nevirapine and HEPT analogues with HIV-1 reverse transcriptase. <i>Molecular Simulation</i> , 2009, 35, 1224-1241.	0.9	4
262	Using a mutual information-based site transition network to map the genetic evolution of influenza A/H3N2 virus. <i>Bioinformatics</i> , 2009, 25, 2309-2317.	1.8	31
263	Free energy simulations reveal a double mutant avian H5N1 virus hemagglutinin with altered receptor binding specificity. <i>Journal of Computational Chemistry</i> , 2009, 30, 1654-1663.	1.5	77
264	Dewetting and Hydrophobic Interaction in Physical and Biological Systems. <i>Annual Review of Physical Chemistry</i> , 2009, 60, 85-103.	4.8	423
265	Recognition Mechanism of siRNA by Viral p19 Suppressor of RNA Silencing: A Molecular Dynamics Study. <i>Biophysical Journal</i> , 2009, 96, 1761-1769.	0.2	19
266	Urea's Action on Hydrophobic Interactions. <i>Journal of the American Chemical Society</i> , 2009, 131, 1535-1541.	6.6	288
267	Sequence-based protein domain boundary prediction using BP neural network with various property profiles. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 71, 300-307.	1.5	9
268	Single Mutation Induced H3N2 Hemagglutinin Antibody Neutralization: A Free Energy Perturbation Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 15813-15820.	1.2	76
269	Role of Water in Mediating the Assembly of Alzheimer Amyloid- β 16-22 Protofilaments. <i>Journal of the American Chemical Society</i> , 2008, 130, 11066-11072.	6.6	208
270	Urea denaturation by stronger dispersion interactions with proteins than water implies a 2-stage unfolding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 16928-16933.	3.3	470

#	ARTICLE	IF	CITATIONS
271	Replica Exchange Molecular Dynamics Method for Protein Folding Simulation. , 2007, 350, 205-224.		62
272	Electrostatic gating of a nanometer water channel. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 3687-3692.	3.3	295
273	Destruction of long-range interactions by a single mutation in lysozyme. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 5824-5829.	3.3	71
274	PROTERAN: animated terrain evolution for visual analysis of patterns in protein folding trajectory. Bioinformatics, 2007, 23, 99-106.	1.8	14
275	Single-mutation-induced stability loss in protein lysozyme. Biochemical Society Transactions, 2007, 35, 1551-1557.	1.6	12
276	Nanoscale Dewetting Transition in Protein Complex Folding. Journal of Physical Chemistry B, 2007, 111, 9069-9077.	1.2	78
277	Replica Exchange with Solute Tempering: Efficiency in Large Scale Systems. Journal of Physical Chemistry B, 2007, 111, 5405-5410.	1.2	103
278	Thermal Denaturing of Mutant Lysozyme with Both the OPLSAA and the CHARMM Force Fields. Journal of the American Chemical Society, 2006, 128, 13388-13395.	6.6	76
279	Hydrophobic Aided Replica Exchange: an Efficient Algorithm for Protein Folding in Explicit Solvent. Journal of Physical Chemistry B, 2006, 110, 19018-19022.	1.2	74
280	Hydration and Dewetting near Fluorinated Superhydrophobic Plates. Journal of the American Chemical Society, 2006, 128, 12439-12447.	6.6	66
281	Dynamics of Water Confined in the Interdomain Region of a Multidomain Protein. Journal of Physical Chemistry B, 2006, 110, 3704-3711.	1.2	93
282	Magnitude and spatial orientation of the hydrophobic moments of multi-domain proteins. International Journal of Bioinformatics Research and Applications, 2006, 2, 161.	0.1	2
283	Is Poisson-Boltzmann theory insufficient for protein folding simulations?. Journal of Chemical Physics, 2006, 124, 034902.	1.2	44
284	A combined steepest descent and genetic algorithm (SD/GA) approach for the optimization of solvation parameters. Molecular Simulation, 2006, 32, 427-435.	0.9	5
285	Blue Matter: Strong Scaling of Molecular Dynamics on Blue Gene/L. Lecture Notes in Computer Science, 2006, , 846-854.	1.0	38
286	Protein Folding with the Parallel Replica Exchange Molecular Dynamics Method. , 2005, , 395-425.		0
287	Observation of a dewetting transition in the collapse of the melittin tetramer. Nature, 2005, 437, 159-162.	13.7	362
288	Hydration and Dewetting near Graphite-CH ₃ and Graphite-COOH Plates. Journal of Physical Chemistry B, 2005, 109, 13639-13648.	1.2	74

#	ARTICLE	IF	CITATIONS
289	Drying and Hydrophobic Collapse of Paraffin Plates. <i>Journal of Physical Chemistry B</i> , 2005, 109, 3546-3552.	1.2	71
290	A WAVELET APPROACH FOR THE ANALYSIS OF FOLDING TRAJECTORY OF PROTEIN TRP-CAGE. <i>Journal of Bioinformatics and Computational Biology</i> , 2005, 03, 1351-1370.	0.3	6
291	Combinatorial Pattern Discovery Approach for the Folding Trajectory Analysis of a $\hat{\Gamma}^2$ -Hairpin. <i>PLoS Computational Biology</i> , 2005, 1, e8.	1.5	4
292	Exploring the protein folding free energy landscape: coupling replica exchange method with P3ME/RESPA algorithm. <i>Journal of Molecular Graphics and Modelling</i> , 2004, 22, 451-463.	1.3	69
293	Hydrophobic Collapse in Multidomain Protein Folding. <i>Science</i> , 2004, 305, 1605-1609.	6.0	482
294	Comment on "Can a Continuum Solvent Model Reproduce the Free Energy Landscape of a $\hat{\Gamma}^2$ -Hairpin Folding in Water?" The Poisson-Boltzmann Equation. <i>Journal of Physical Chemistry B</i> , 2004, 108, 7528-7530.	1.2	34
295	Describing Protein Folding Kinetics by Molecular Dynamics Simulations. 2. Example Applications to Alanine Dipeptide and a $\hat{\Gamma}^2$ -Hairpin Peptide. <i>Journal of Physical Chemistry B</i> , 2004, 108, 6582-6594.	1.2	171
296	A computationally inexpensive modification of the point dipole electrostatic polarization model for molecular simulations. <i>Journal of Computational Chemistry</i> , 2003, 24, 267-276.	1.5	56
297	Blue Matter, an application framework for molecular simulation on Blue Gene. <i>Journal of Parallel and Distributed Computing</i> , 2003, 63, 759-773.	2.7	62
298	Spatial profiling of protein hydrophobicity: Native vs. Decoy structures. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003, 52, 561-572.	1.5	23
299	Free energy landscape of protein folding in water: Explicit vs. implicit solvent. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003, 53, 148-161.	1.5	284
300	Trp-cage: Folding free energy landscape in explicit water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2003, 100, 13280-13285.	3.3	347
301	Can a continuum solvent model reproduce the free energy landscape of a $\hat{\Gamma}$ -hairpin folding in water?. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 12777-12782.	3.3	326
302	Development of a polarizable force field for proteins via ab initio quantum chemistry: First generation model and gas phase tests. <i>Journal of Computational Chemistry</i> , 2002, 23, 1515-1531.	1.5	296
303	Blue Gene: A vision for protein science using a petaflop supercomputer. <i>IBM Systems Journal</i> , 2001, 40, 310-327.	3.1	211
304	New Linear Interaction Method for Binding Affinity Calculations Using a Continuum Solvent Model. <i>Journal of Physical Chemistry B</i> , 2001, 105, 10388-10397.	1.2	124
305	The free energy landscape for $\hat{\Gamma}$ hairpin folding in explicit water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2001, 98, 14931-14936.	3.3	499
306	Efficient multiple time step method for use with Ewald and particle mesh Ewald for large biomolecular systems. <i>Journal of Chemical Physics</i> , 2001, 115, 2348-2358.	1.2	121

#	ARTICLE	IF	CITATIONS
307	Poisson-Boltzmann Analytical Gradients for Molecular Modeling Calculations. Journal of Physical Chemistry B, 1999, 103, 3057-3061.	1.2	146
308	Parametrizing a polarizable force field from ab initio data. I. The fluctuating point charge model. Journal of Chemical Physics, 1999, 110, 741-754.	1.2	251
309	Fluctuating Charge, Polarizable Dipole, and Combined Models: Parameterization from ab Initio Quantum Chemistry. Journal of Physical Chemistry B, 1999, 103, 4730-4737.	1.2	250
310	Large scale simulation of macromolecules in solution: Combining the periodic fast multipole method with multiple time step integrators. Journal of Chemical Physics, 1997, 106, 9835-9849.	1.2	108
311	Smart walking: A new method for Boltzmann sampling of protein conformations. Journal of Chemical Physics, 1997, 107, 9185-9196.	1.2	87
312	Molecular dynamics with multiple time scales: The selection of efficient reference system propagators. Journal of Chemical Physics, 1996, 105, 1426-1436.	1.2	121
313	Molecular dynamics for nonequilibrium systems in which there are a small number of very hot particles in a cold bath: Reference system propagator methods. Journal of Chemical Physics, 1996, 105, 235-239.	1.2	4
314	A new molecular dynamics method combining the reference system propagator algorithm with a fast multipole method for simulating proteins and other complex systems. Journal of Chemical Physics, 1995, 103, 9444-9459.	1.2	96
315	Condensed Matter, 1994, 6, 6103-6109.	0.7	18
316	Ethylene adsorption and decomposition on Si(100) 2*1: a semi-empirical quantum chemical study. Journal of Physics Condensed Matter, 1993, 5, 2887-2896.	0.7	17
317	The bonding characterization of Br on Si(100)2*1. Journal of Physics Condensed Matter, 1993, 5, 2897-2902.	0.7	6
318	Total-energy calculations for acetylene adsorption and decomposition on Si(100)-2x1. Physical Review B, 1993, 47, 10601-10606.	1.1	33
319	pi-bonded N2 on Cr(110) as a precursor for dissociation: molecular orbital theory. Journal of Physics Condensed Matter, 1992, 4, 2429-2437.	0.7	6
320	Molecular cluster analysis of O2 adsorption and dissociation on Pt(111). Physics Letters, Section A: General, Atomic and Solid State Physics, 1992, 169, 167-172.	0.9	10
321	Small Molecules and Peptides Inside Carbon Nanotubes: Impact of Nanoscale Confinement. , 0, , .		2