Ruhong Zhou

List of Publications by Year
in descending order

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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	Destructive extraction of phospholipids from Escherichia coli membranes by graphene nanosheets. Nature Nanotechnology, 2013, 8, 594-601.	15.6	1,260
2	Binding of blood proteins to carbon nanotubes reduces cytotoxicity. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 16968-16973.	3.3	839
3	Patient HLA class I genotype influences cancer response to checkpoint blockade immunotherapy. Science, 2018, 359, 582-587.	6.0	834
4	The free energy landscape for Â hairpin folding in explicit water. Proceedings of the National Academy of Sciences of the United States of America, 2001, 98, 14931-14936.	3.3	499
5	Hydrophobic Collapse in Multidomain Protein Folding. Science, 2004, 305, 1605-1609.	6.0	482
6	Urea denaturation by stronger dispersion interactions with proteins than water implies a 2-stage unfolding. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 16928-16933.	3.3	470
7	Dewetting and Hydrophobic Interaction in Physical and Biological Systems. Annual Review of Physical Chemistry, 2009, 60, 85-103.	4.8	423
8	Differential Pd-nanocrystal facets demonstrate distinct antibacterial activity against Gram-positive and Gram-negative bacteria. Nature Communications, 2018, 9, 129.	5.8	414
9	Identifying the Recognition Site for Selective Trapping of ⁹⁹TcO₄^{â€“} in a Hydrolytically Stable and Radiation Resistant Cationic Metalâ€“Organic Framework. Journal of the American Chemical Society, 2017, 139, 14873-14876.	6.6	386
10	Overcoming the crystallization and designability issues in the ultrastable zirconium phosphonate framework system. Nature Communications, 2017, 8, 15369.	5.8	366
11	Observation of a dewetting transition in the collapse of the melittin tetramer. Nature, 2005, 437, 159-162.	13.7	362
12	Trp-cage: Folding free energy landscape in explicit water. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 13280-13285.	3.3	347
13	Half a century of amyloids: past, present and future. Chemical Society Reviews, 2020, 49, 5473-5509.	18.7	345
14	Highly Sensitive and Selective Uranium Detection in Natural Water Systems Using a Luminescent Mesoporous Metalâ€“Organic Framework Equipped with Abundant Lewis Basic Sites: A Combined Batch, X-ray Absorption Spectroscopy, and First Principles Simulation Investigation. Environmental Science & Technology, 2017, 51, 3911-3921.	4.6	331
15	Can a continuum solvent model reproduce the free energy landscape of a Â-hairpin folding in water?. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 12777-12782.	3.3	326
16	Development of a polarizable force field for proteins via ab initio quantum chemistry: First generation model and gas phase tests. Journal of Computational Chemistry, 2002, 23, 1515-1531.	1.5	296
17	A mesoporous cationic thorium-organic framework that rapidly traps anionic persistent organic pollutants. Nature Communications, 2017, 8, 1354.	5.8	296
18	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

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19	Comprehensive interrogation of natural TALE DNA-binding modules and transcriptional repressor domains. Nature Communications, 2012, 3, 968.	5.8	291
20	Ureaâ€™s Action on Hydrophobic Interactions. Journal of the American Chemical Society, 2009, 131, 1535-1541.	6.6	288
21	Free energy landscape of protein folding in water: Explicit vs. implicit solvent. Proteins: Structure, Function and Bioinformatics, 2003, 53, 148-161.	1.5	284
22	Reduced Cytotoxicity of Graphene Nanosheets Mediated by Blood-Protein Coating. ACS Nano, 2015, 9, 5713-5724.	7.3	271
23	Probing the Self-Assembly Mechanism of Diphenylalanine-Based Peptide Nanovesicles and Nanotubes. ACS Nano, 2012, 6, 3907-3918.	7.3	264
24	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
25	Fluctuating Charge, Polarizable Dipole, and Combined Models:â€‰ Parameterization from ab Initio Quantum Chemistry. Journal of Physical Chemistry B, 1999, 103, 4730-4737.	1.2	250
26	Degradable Carbon Dots with Broad-Spectrum Antibacterial Activity. ACS Applied Materials & Interfaces, 2018, 10, 26936-26946.	4.0	246
27	Tunable, Strain-Controlled Nanoporous MoS₂ Filter for Water Desalination. ACS Nano, 2016, 10, 1829-1835.	7.3	212
28	Blue Gene: A vision for protein science using a petaflop supercomputer. IBM Systems Journal, 2001, 40, 310-327.	3.1	211
29	Role of Water in Mediating the Assembly of Alzheimer Amyloid-Î² AÎ²16â^'22 Protofilaments. Journal of the American Chemical Society, 2008, 130, 11066-11072.	6.6	208
30	Protein corona mitigates the cytotoxicity of graphene oxide by reducing its physical interaction with cell membrane. Nanoscale, 2015, 7, 15214-15224.	2.8	204
31	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
32	Adsorption of Villin Headpiece onto Graphene, Carbon Nanotube, and C60: Effect of Contacting Surface Curvatures on Binding Affinity. Journal of Physical Chemistry C, 2011, 115, 23323-23328.	1.5	181
33	Exceptional Perrhenate/Pertechnetate Uptake and Subsequent Immobilization by a Low-Dimensional Cationic Coordination Polymer: Overcoming the Hofmeister Bias Selectivity. Environmental Science and Technology Letters, 2017, 4, 316-322.	3.9	181
34	Unique Proton Transportation Pathway in a Robust Inorganic Coordination Polymer Leading to Intrinsically High and Sustainable Anhydrous Proton Conductivity. Journal of the American Chemical Society, 2018, 140, 6146-6155.	6.6	181
35	Mechanism unravelling for ultrafast and selective ⁹⁹TcO₄^{â^'} uptake by a radiation-resistant cationic covalent organic framework: a combined radiological experiment and molecular dynamics simulation study. Chemical Science, 2019, 10, 4293-4305.	3.7	181
36	Successful Decontamination of ⁹⁹TcO₄^{â^'} in Groundwater at Legacy Nuclear Sites by a Cationic Metalâ€Organic Framework with Hydrophobic Pockets. Angewandte Chemie - International Edition, 2019, 58, 4968-4972.	7.2	177

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37	Describing Protein Folding Kinetics by Molecular Dynamics Simulations. 2. Example Applications to Alanine Dipeptide and a Î²-Hairpin Peptide. Journal of Physical Chemistry B, 2004, 108, 6582-6594.	1.2	171
38	Plugging into Proteins: Poisoning Protein Function by a Hydrophobic Nanoparticle. ACS Nano, 2010, 4, 7508-7514.	7.3	168
39	Potential Toxicity of Graphene to Cell Functions via Disrupting Proteinâ€“Protein Interactions. ACS Nano, 2015, 9, 663-669.	7.3	164
40	PEGylated graphene oxide elicits strong immunological responses despite surface passivation. Nature Communications, 2017, 8, 14537.	5.8	157
41	Poissonâ^'Boltzmann Analytical Gradients for Molecular Modeling Calculations. Journal of Physical Chemistry B, 1999, 103, 3057-3061.	1.2	146
42	Opening Lids: Modulation of Lipase Immobilization by Graphene Oxides. ACS Catalysis, 2016, 6, 4760-4768.	5.5	139
43	Towards understanding of nanoparticleâ€“protein corona. Archives of Toxicology, 2015, 89, 519-539.	1.9	135
44	Interactions Between Proteins and Carbonâ€Based Nanoparticles: Exploring the Origin of Nanotoxicity at the Molecular Level. Small, 2013, 9, 1546-1556.	5.2	132
45	New Linear Interaction Method for Binding Affinity Calculations Using a Continuum Solvent Model. Journal of Physical Chemistry B, 2001, 105, 10388-10397.	1.2	124
46	99TcO4â^' removal from legacy defense nuclear waste by an alkaline-stable 2D cationic metal organic framework. Nature Communications, 2020, 11, 5571.	5.8	124
47	Molecular dynamics with multiple time scales: The selection of efficient reference system propagators. Journal of Chemical Physics, 1996, 105, 1426-1436.	1.2	121
48	Efficient multiple time step method for use with Ewald and particle mesh Ewald for large biomolecular systems. Journal of Chemical Physics, 2001, 115, 2348-2358.	1.2	121
49	Water-mediated signal multiplication with Y-shaped carbon nanotubes. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 18120-18124.	3.3	120
50	Aggregation of Î³-crystallins associated with human cataracts via domain swapping at the C-terminal Î²-strands. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 10514-10519.	3.3	117
51	Wettability and friction of water on a MoS2 nanosheet. Applied Physics Letters, 2016, 108, .	1.5	113
52	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
53	A 3,2-Hydroxypyridinone-based Decorporation Agent that Removes Uranium from Bones In Vivo. Nature Communications, 2019, 10, 2570.	5.8	107
54	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

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55	Replica Exchange with Solute Tempering:Â Efficiency in Large Scale Systems. Journal of Physical Chemistry B, 2007, 111, 5405-5410.	1.2	103
56	Amino acid analogues bind to carbon nanotube via Ï€-Ï€ interactions: Comparison of molecular mechanical and quantum mechanical calculations. Journal of Chemical Physics, 2012, 136, 025103.	1.2	103
57	Graphene-Induced Pore Formation on Cell Membranes. Scientific Reports, 2017, 7, 42767.	1.6	103
58	A Public BCR Present in a Unique Dual-Receptor-Expressing Lymphocyte from Type 1 Diabetes Patients Encodes a Potent T Cell Autoantigen. Cell, 2019, 177, 1583-1599.e16.	13.5	103
59	Cytotoxicity of graphene: recent advances and future perspective. Wiley Interdisciplinary Reviews: Nanomedicine and Nanobiotechnology, 2014, 6, 452-474.	3.3	101
60	Destruction of amyloid fibrils by graphene through penetration and extraction of peptides. Nanoscale, 2015, 7, 18725-18737.	2.8	101
61	Triphenylalanine peptides self-assemble into nanospheres and nanorods that are different from the nanovesicles and nanotubes formed by diphenylalanine peptides. Nanoscale, 2014, 6, 2800.	2.8	100
62	Surface Curvature Relation to Protein Adsorption for Carbon-based Nanomaterials. Scientific Reports, 2015, 5, 10886.	1.6	97
63	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
64	Commensal bacteria stimulate antitumor responses via T cell cross-reactivity. JCI Insight, 2020, 5, .	2.3	95
65	Dynamics of Water Confined in the Interdomain Region of a Multidomain Proteinâ€. Journal of Physical Chemistry B, 2006, 110, 3704-3711.	1.2	93
66	Electron Beam Irradiation as a General Approach for the Rapid Synthesis of Covalent Organic Frameworks under Ambient Conditions. Journal of the American Chemical Society, 2020, 142, 9169-9174.	6.6	90
67	The role of basic residues in the adsorption of blood proteins onto the graphene surface. Scientific Reports, 2015, 5, 10873.	1.6	88
68	Smart walking: A new method for Boltzmann sampling of protein conformations. Journal of Chemical Physics, 1997, 107, 9185-9196.	1.2	87
69	Palladium concave nanocrystals with high-index facets accelerate ascorbate oxidation in cancer treatment. Nature Communications, 2018, 9, 4861.	5.8	84
70	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
71	Hydrated Excess Protons Can Create Their Own Water Wires. Journal of Physical Chemistry B, 2015, 119, 9212-9218.	1.2	83
72	Complete wetting of graphene by biological lipids. Nanoscale, 2016, 8, 5750-5754.	2.8	83

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73	A Peptide-Coated Gold Nanocluster Exhibits Unique Behavior in Protein Activity Inhibition. Journal of the American Chemical Society, 2015, 137, 8412-8418.	6.6	79
74	Hydroxyl-Group-Dominated Graphite Dots Reshape Laser Desorption/Ionization Mass Spectrometry for Small Biomolecular Analysis and Imaging. ACS Nano, 2017, 11, 9500-9513.	7.3	79
75	Nanoscale Dewetting Transition in Protein Complex Folding. Journal of Physical Chemistry B, 2007, 111, 9069-9077.	1.2	78
76	Free energy simulations reveal a double mutant avian H5N1 virus hemagglutinin with altered receptor binding specificity. Journal of Computational Chemistry, 2009, 30, 1654-1663.	1.5	77
77	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
78	Single Mutation Induced H3N2 Hemagglutinin Antibody Neutralization: A Free Energy Perturbation Study. Journal of Physical Chemistry B, 2008, 112, 15813-15820.	1.2	76
79	Membrane destruction-mediated antibacterial activity of tungsten disulfide (WS₂). RSC Advances, 2017, 7, 37873-37880.	1.7	76
80	Hydration and Dewetting near Graphiteâ^'CH3and Graphiteâ^'COOH Plates. Journal of Physical Chemistry B, 2005, 109, 13639-13648.	1.2	74
81	Hydrophobic Aided Replica Exchange:Â an Efficient Algorithm for Protein Folding in Explicit Solventâ€. Journal of Physical Chemistry B, 2006, 110, 19018-19022.	1.2	74
82	Robust Antibacterial Activity of Tungsten Oxide (WO_{3-x}) Nanodots. Chemical Research in Toxicology, 2019, 32, 1357-1366.	1.7	73
83	Drying and Hydrophobic Collapse of Paraffin Plates. Journal of Physical Chemistry B, 2005, 109, 3546-3552.	1.2	71
84	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
85	Exploring the protein folding free energy landscape: coupling replica exchange method with P3ME/RESPA algorithm. Journal of Molecular Graphics and Modelling, 2004, 22, 451-463.	1.3	69
86	Graphene Oxide Nanosheets Retard Cellular Migration via Disruption of Actin Cytoskeleton. Small, 2017, 13, 1602133.	5.2	68
87	Hydration and Dewetting near Fluorinated Superhydrophobic Plates. Journal of the American Chemical Society, 2006, 128, 12439-12447.	6.6	66
88	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. PLoS Medicine, 2015, 12, e1001900.	3.9	66
89	Revealing the importance of surface morphology of nanomaterials to biological responses: Adsorption of the villin headpiece onto graphene and phosphorene. Carbon, 2015, 94, 895-902.	5.4	65
90	Gdâ€"Metallofullerenol Nanomaterial Suppresses Pancreatic Cancer Metastasis by Inhibiting the Interaction of Histone Deacetylase 1 and Metastasis-Associated Protein 1. ACS Nano, 2015, 9, 6826-6836.	7.3	64

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91	High-Curvature Nanostructuring Enhances Probe Display for Biomolecular Detection. Nano Letters, 2017, 17, 1289-1295.	4.5	64
92	Blue Matter, an application framework for molecular simulation on Blue Gene. Journal of Parallel and Distributed Computing, 2003, 63, 759-773.	2.7	62
93	Replica Exchange Molecular Dynamics Method for Protein Folding Simulation. , 2007, 350, 205-224.		62
94	Molecular dynamics simulations of Ago silencing complexes reveal a large repertoire of admissible â€˜seed-lessâ€™ targets. Scientific Reports, 2012, 2, 569.	1.6	62
95	Stability of Ligands on Nanoparticles Regulating the Integrity of Biological Membranes at the Nanoâ€“Lipid Interface. ACS Nano, 2019, 13, 8680-8693.	7.3	59
96	Urea-Induced Drying of Carbon Nanotubes Suggests Existence of a Dry Globule-like Transient State During Chemical Denaturation of Proteins. Journal of Physical Chemistry B, 2010, 114, 5427-5430.	1.2	58
97	Molecular Dynamics with Multiple Time Scales: How to Avoid Pitfalls. Journal of Chemical Theory and Computation, 2010, 6, 1798-1804.	2.3	57
98	Spontaneous Transport of Single-Stranded DNA through Grapheneâ€“MoS₂ Heterostructure Nanopores. ACS Nano, 2018, 12, 3886-3891.	7.3	57
99	A computationally inexpensive modification of the point dipole electrostatic polarization model for molecular simulations. Journal of Computational Chemistry, 2003, 24, 267-276.	1.5	56
100	Carbon Nanotube Wins the Competitive Binding over Proline-Rich Motif Ligand on SH3 Domain. Journal of Physical Chemistry C, 2011, 115, 12322-12328.	1.5	56
101	Hydrophobic Interaction Drives Surface-Assisted Epitaxial Assembly of Amyloid-like Peptides. Journal of the American Chemical Society, 2013, 135, 3150-3157.	6.6	56
102	Nanomedicine: de novo design of nanodrugs. Nanoscale, 2014, 6, 663-677.	2.8	56
103	Emergence of a Radicalâ€Stabilizing Metalâ€“Organic Framework as a Radioâ€photoluminescence Dosimeter. Angewandte Chemie - International Edition, 2020, 59, 15209-15214.	7.2	56
104	Collapse of Unfolded Proteins in a Mixture of Denaturants. Journal of the American Chemical Society, 2012, 134, 18266-18274.	6.6	55
105	Polymeric prodrugs conjugated with reduction-sensitive dextranâ€“camptothecin and pH-responsive dextranâ€“doxorubicin: an effective combinatorial drug delivery platform for cancer therapy. Polymer Chemistry, 2016, 7, 4198-4212.	1.9	53
106	Urea-Induced Drying of Hydrophobic Nanotubes: Comparison of Different Urea Models. Journal of Physical Chemistry B, 2011, 115, 2988-2994.	1.2	52
107	Highly Sensitive Detection of UV Radiation Using a Uranium Coordination Polymer. ACS Applied Materials & Interfaces, 2018, 10, 4844-4850.	4.0	52
108	Orientational Binding of DNA Guided by the C₂N Template. ACS Nano, 2017, 11, 3198-3206.	7.3	51

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109	Exploration of graphene oxide as an intelligent platform for cancer vaccines. Nanoscale, 2015, 7, 19949-19957.	2.8	49
110	DNA translocation through single-layer boron nitride nanopores. Soft Matter, 2016, 12, 817-823.	1.2	49
111	In silico design and validation of high-affinity RNA aptamers targeting epithelial cellular adhesion molecule dimers. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 8486-8493.	3.3	49
112	A new molecular mechanism underlying the EGCG-mediated autophagic modulation of AFP in HepG2 cells. Cell Death and Disease, 2017, 8, e3160-e3160.	2.7	48
113	Self-Assembled Coreâ€“Satellite Gold Nanoparticle Networks for Ultrasensitive Detection of Chiral Molecules by Recognition Tunneling Current. ACS Nano, 2016, 10, 5096-5103.	7.3	47
114	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
115	A Porous Aromatic Framework Functionalized with Luminescent Iridium(III) Organometallic Complexes for Turn-On Sensing of ⁹⁹TcO₄^{â€“}. ACS Applied Materials & Interfaces, 2020, 12, 15288-15297.	4.0	46
116	Single-File Protein Translocations through Grapheneâ€“MoS₂ Heterostructure Nanopores. Journal of Physical Chemistry Letters, 2018, 9, 3409-3415.	2.1	45
117	Is Poisson-Boltzmann theory insufficient for protein folding simulations?. Journal of Chemical Physics, 2006, 124, 034902.	1.2	44
118	Exploring the Nanotoxicology of MoS₂: A Study on the Interaction of MoS₂ Nanoflakes and K⁺ Channels. ACS Nano, 2018, 12, 705-717.	7.3	44
119	Single-Walled Carbon Nanotubes Inhibit the Cytochrome P450 Enzyme, CYP3A4. Scientific Reports, 2016, 6, 21316.	1.6	43
120	Emerging Î²-Sheet Rich Conformations in Supercompact Huntingtin Exon-1 Mutant Structures. Journal of the American Chemical Society, 2017, 139, 8820-8827.	6.6	43
121	Structural influence of proteins upon adsorption to MoS₂ nanomaterials: comparison of MoS₂ force field parameters. Physical Chemistry Chemical Physics, 2017, 19, 3039-3045.	1.3	43
122	Lanosterol Disrupts Aggregation of Human Î³D-Crystallin by Binding to the Hydrophobic Dimerization Interface. Journal of the American Chemical Society, 2018, 140, 8479-8486.	6.6	42
123	Non-destructive Inhibition of Metallofullerenol Gd@C82(OH)22 on WW domain: Implication on Signal Transduction Pathway. Scientific Reports, 2012, 2, 957.	1.6	41
124	Simplified TiO2 force fields for studies of its interaction with biomolecules. Journal of Chemical Physics, 2015, 142, 234102.	1.2	41
125	Stimulating antibacterial activities of graphitic carbon nitride nanosheets with plasma treatment. Nanoscale, 2019, 11, 18416-18425.	2.8	41
126	An In Silico study of TiO2 nanoparticles interaction with twenty standard amino acids in aqueous solution. Scientific Reports, 2016, 6, 37761.	1.6	40

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127	Structural Damage of a Î²-Sheet Protein upon Adsorption onto Molybdenum Disulfide Nanotubes. Journal of Physical Chemistry C, 2016, 120, 6796-6803.	1.5	39
128	Î²â€strand interactions at the domain interface critical for the stability of human lens Î³Dâ€crystallin. Protein Science, 2010, 19, 131-140.	3.1	38
129	Salting Effects on Protein Components in Aqueous NaCl and Urea Solutions: Toward Understanding of Urea-Induced Protein Denaturation. Journal of Physical Chemistry B, 2012, 116, 1446-1451.	1.2	38
130	Blue Matter: Strong Scaling of Molecular Dynamics on Blue Gene/L. Lecture Notes in Computer Science, 2006, , 846-854.	1.0	38
131	UV-radiation Induced Disruption of Dry-Cavities in Human Î³D-crystallin Results in Decreased Stability and Faster Unfolding. Scientific Reports, 2013, 3, 1560.	1.6	37
132	Exploring biological effects of MoS2 nanosheets on native structures of Î±-helical peptides. Journal of Chemical Physics, 2016, 144, 175103.	1.2	37
133	Mild Binding of Protein to C₂N Monolayer Reveals Its Suitable Biocompatibility. Small, 2017, 13, 1603685.	5.2	37
134	Successful Decontamination of ⁹⁹TcO₄^{â^'} in Groundwater at Legacy Nuclear Sites by a Cationic Metalâ€Organic Framework with Hydrophobic Pockets. Angewandte Chemie, 2019, 131, 5022-5026.	1.6	37
135	Spontaneous ssDNA stretching on graphene and hexagonal boron nitride in plane heterostructures. Nature Communications, 2019, 10, 4610.	5.8	36
136	Comment on â€œUrea-Mediated Protein Denaturation: A Consensus Viewâ€• Journal of Physical Chemistry B, 2011, 115, 1323-1326.	1.2	35
137	Phase transition triggered aggregation-induced emission in a photoluminescent uranylâ€“organic framework. Chemical Communications, 2018, 54, 627-630.	2.2	35
138	The molecular mechanism of robust macrophage immune responses induced by PEGylated molybdenum disulfide. Nanoscale, 2019, 11, 22293-22304.	2.8	35
139	Comment on â€œCan a Continuum Solvent Model Reproduce the Free Energy Landscape of a Î²-Hairpin Folding in Water?â€•The Poissonâ^'Boltzmann Equation. Journal of Physical Chemistry B, 2004, 108, 7528-7530.	1.2	34
140	Characterization of a Novel Water Pocket Inside the Human Cx26 Hemichannel Structure. Biophysical Journal, 2014, 107, 599-612.	0.2	34
141	Large scale molecular simulations of nanotoxicity. Wiley Interdisciplinary Reviews: Systems Biology and Medicine, 2014, 6, 329-343.	6.6	34
142	Total-energy calculations for acetylene adsorption and decomposition on Si(100)-2Ã—1. Physical Review B, 1993, 47, 10601-10606.	1.1	33
143	Single Mutation Effects on Conformational Change and Membrane Deformation of Influenza Hemagglutinin Fusion Peptides. Journal of Physical Chemistry B, 2010, 114, 8799-8806.	1.2	33
144	Signal transmission, conversion and multiplication by polar molecules confined in nanochannels. Nanoscale, 2010, 2, 1976.	2.8	33

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145	Dynamics of DNA translocation in a solid-state nanopore immersed in aqueous glycerol. Nanotechnology, 2012, 23, 455102.	1.3	33
146	Robust Denaturation of Villin Headpiece by MoS2 Nanosheet: Potential Molecular Origin of the Nanotoxicity. Scientific Reports, 2016, 6, 28252.	1.6	33
147	Hydrogen and methane storage and release by MoS₂ nanotubes for energy storage. Journal of Materials Chemistry A, 2017, 5, 23020-23027.	5.2	33
148	Superior Compatibility of C₂N with Human Red Blood Cell Membranes and the Underlying Mechanism. Small, 2018, 14, e1803509.	5.2	33
149	Facile and Efficient Decontamination of Thorium from Rare Earths Based on Selective Selenite Crystallization. Inorganic Chemistry, 2018, 57, 1880-1887.	1.9	32
150	Using a mutual information-based site transition network to map the genetic evolution of influenza A/H3N2 virus. Bioinformatics, 2009, 25, 2309-2317.	1.8	31
151	Membrane Insertion and Phospholipids Extraction by Graphyne Nanosheets. Journal of Physical Chemistry C, 2017, 121, 2444-2450.	1.5	31
152	Combined Computationalâ€“Experimental Approach to Explore the Molecular Mechanism of SaCas9 with a Broadened DNA Targeting Range. Journal of the American Chemical Society, 2019, 141, 6545-6552.	6.6	31
153	Atomic-Scale Fluidic Diodes Based on Triangular Nanopores in Bilayer Hexagonal Boron Nitride. Nano Letters, 2019, 19, 977-982.	4.5	31
154	Self-cascade MoS₂ nanozymes for efficient intracellular antioxidation and hepatic fibrosis therapy. Nanoscale, 2021, 13, 12613-12622.	2.8	31
155	Enantiomerization Mechanism of Thalidomide and the Role of Water and Hydroxide Ions. Chemistry - A European Journal, 2012, 18, 14305-14313.	1.7	30
156	Free-Energy Simulations Reveal that Both Hydrophobic and Polar Interactions Are Important for Influenza Hemagglutinin Antibody Binding. Biophysical Journal, 2012, 102, 1453-1461.	0.2	30
157	Molecular Structure and Dynamics of Water on Pristine and Strained Phosphorene: Wetting and Diffusion at Nanoscale. Scientific Reports, 2016, 6, 38327.	1.6	30
158	Defect-assisted protein HP35 denaturation on graphene. Nanoscale, 2019, 11, 19362-19369.	2.8	30
159	Distinct lipid membrane interaction and uptake of differentially charged nanoplastics in bacteria. Journal of Nanobiotechnology, 2022, 20, 191.	4.2	30
160	Molecular Mechanism of Surface-Assisted Epitaxial Self-Assembly of Amyloid-like Peptides. ACS Nano, 2012, 6, 9276-9282.	7.3	29
161	Coherent Microscopic Picture for Urea-Induced Denaturation of Proteins. Journal of Physical Chemistry B, 2012, 116, 8856-8862.	1.2	29
162	Multiscale modeling of macromolecular biosystems. Briefings in Bioinformatics, 2012, 13, 395-405.	3.2	29

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163	Structural and electronic properties of uranium-encapsulated Au14 cage. Scientific Reports, 2015, 4, 5862.	1.6	29
164	Binding Specificity Determines the Cytochrome P450 3A4 Mediated Enantioselective Metabolism of Metconazole. Journal of Physical Chemistry B, 2018, 122, 1176-1184.	1.2	29
165	The Folding Transition State of Protein L Is Extensive with Nonnative Interactions (and Not Small and) Tj ETQq1 1 0.784314 rgBT /Ove	2.0	28
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