Ruhong Zhou

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312 18,147 67 126 g-index

338 20,858 8.1 7 L-index

#	Paper	IF	Citations
312	Destructive extraction of phospholipids from Escherichia coli membranes by graphene nanosheets. <i>Nature Nanotechnology</i> , 2013 , 8, 594-601	28.7	1008
311	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, 16968-73	11.5	738
310	Patient HLA class I genotype influences cancer response to checkpoint blockade immunotherapy. <i>Science</i> , 2018 , 359, 582-587	33.3	500
309	The free energy landscape for beta hairpin folding in explicit water. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2001 , 98, 14931-6	11.5	458
308	Hydrophobic collapse in multidomain protein folding. <i>Science</i> , 2004 , 305, 1605-9	33.3	441
307	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, 16928-33	11.5	424
306	Dewetting and hydrophobic interaction in physical and biological systems. <i>Annual Review of Physical Chemistry</i> , 2009 , 60, 85-103	15.7	383
305	Observation of a dewetting transition in the collapse of the melittin tetramer. <i>Nature</i> , 2005 , 437, 159-6	2 50.4	333
304	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, 13280-5	11.5	319
303	Can a continuum solvent model reproduce the free energy landscape of a beta -hairpin folding in water?. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002 , 99, 12777	·- 1 1.5	308
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, 1515-31	3.5	276
301	Electrostatic gating of a nanometer water channel. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007 , 104, 3687-92	11.5	274
300	Free energy landscape of protein folding in water: explicit vs. implicit solvent. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003 , 53, 148-61	4.2	270
299	Overcoming the crystallization and designability issues in the ultrastable zirconium phosphonate framework system. <i>Nature Communications</i> , 2017 , 8, 15369	17.4	266
298	Identifying the Recognition Site for Selective Trapping of TcO in a Hydrolytically Stable and Radiation Resistant Cationic Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2017 , 139, 14873-14876	16.4	263
297	Urea's action on hydrophobic interactions. <i>Journal of the American Chemical Society</i> , 2009 , 131, 1535-41	16.4	261
296	Differential Pd-nanocrystal facets demonstrate distinct antibacterial activity against Gram-positive and Gram-negative bacteria. <i>Nature Communications</i> , 2018 , 9, 129	17.4	260

(2020-2012)

295	Comprehensive interrogation of natural TALE DNA-binding modules and transcriptional repressor domains. <i>Nature Communications</i> , 2012 , 3, 968	17.4	257
294	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</i>	10.3	246
293	Fluctuating Charge, Polarizable Dipole, and Combined Models: Parameterization from ab Initio Quantum Chemistry. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 4730-4737	3.4	239
292	Parametrizing a polarizable force field from ab initio data. I. The fluctuating point charge model. Journal of Chemical Physics, 1999, 110, 741-754	3.9	225
291	Reduced Cytotoxicity of Graphene Nanosheets Mediated by Blood-Protein Coating. <i>ACS Nano</i> , 2015 , 9, 5713-24	16.7	216
290	Probing the self-assembly mechanism of diphenylalanine-based peptide nanovesicles and nanotubes. <i>ACS Nano</i> , 2012 , 6, 3907-18	16.7	213
289	A mesoporous cationic thorium-organic framework that rapidly traps anionic persistent organic pollutants. <i>Nature Communications</i> , 2017 , 8, 1354	17.4	211
288	Role of water in mediating the assembly of Alzheimer amyloid-beta Abeta16-22 protofilaments. Journal of the American Chemical Society, 2008 , 130, 11066-72	16.4	180
287	Molecular mechanism of pancreatic tumor metastasis inhibition by Gd@C82(OH)22 and its implication for de novo design of nanomedicine. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012 , 109, 15431-6	11.5	177
286	Blue Gene: A vision for protein science using a petaflop supercomputer. <i>IBM Systems Journal</i> , 2001 , 40, 310-327		175
285	Tunable, Strain-Controlled Nanoporous MoSIFilter for Water Desalination. ACS Nano, 2016, 10, 1829-35	16.7	174
284	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	3.8	162
283	Describing Protein Folding Kinetics by Molecular Dynamics Simulations. 2. Example Applications to Alanine Dipeptide and a \(\mathre{H}\)airpin Peptide\(\Display \) Journal of Physical Chemistry B, 2004 , 108, 6582-6594	3.4	159
282	Protein corona mitigates the cytotoxicity of graphene oxide by reducing its physical interaction with cell membrane. <i>Nanoscale</i> , 2015 , 7, 15214-24	7.7	157
281	Plugging into proteins: poisoning protein function by a hydrophobic nanoparticle. <i>ACS Nano</i> , 2010 , 4, 7508-14	16.7	155
280	Potential toxicity of graphene to cell functions via disrupting protein-protein interactions. <i>ACS Nano</i> , 2015 , 9, 663-9	16.7	143
279	Degradable Carbon Dots with Broad-Spectrum Antibacterial Activity. <i>ACS Applied Materials & Amp; Interfaces</i> , 2018 , 10, 26936-26946	9.5	143
278	Half a century of amyloids: past, present and future. <i>Chemical Society Reviews</i> , 2020 , 49, 5473-5509	58.5	142

277	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	16.4	133
276	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	11	131
275	PEGylated graphene oxide elicits strong immunological responses despite surface passivation. <i>Nature Communications</i> , 2017 , 8, 14537	17.4	120
274	Poisson B oltzmann Analytical Gradients for Molecular Modeling Calculations. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 3057-3061	3.4	120
273	New Linear Interaction Method for Binding Affinity Calculations Using a Continuum Solvent Model. Journal of Physical Chemistry B, 2001 , 105, 10388-10397	3.4	116
272	Interactions between proteins and carbon-based nanoparticles: exploring the origin of nanotoxicity at the molecular level. <i>Small</i> , 2013 , 9, 1546-56	11	113
271	Towards understanding of nanoparticle-protein corona. <i>Archives of Toxicology</i> , 2015 , 89, 519-39	5.8	112
270	Successful Decontamination of TcO 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	16.4	111
269	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, 18120-4	11.5	109
268	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	3.9	104
267	Opening Lids: Modulation of Lipase Immobilization by Graphene Oxides. ACS Catalysis, 2016 , 6, 4760-47	768 .1	103
266	Aggregation of Erystallins associated with human cataracts via domain swapping at the C-terminal Batrands. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011 , 108, 10514-9	11.5	100
265	Large scale simulation of macromolecules in solution: Combining the periodic fast multipole method with multiple time step integrators. <i>Journal of Chemical Physics</i> , 1997 , 106, 9835-9849	3.9	98
264	Mechanism unravelling for ultrafast and selective TcO 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	9.4	96
263	Replica exchange with solute tempering: efficiency in large scale systems. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 5405-10	3.4	95
262	Dynamics of water confined in the interdomain region of a multidomain protein. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 3704-11	3.4	88
261	Molecular dynamics with multiple time scales: The selection of efficient reference system propagators. <i>Journal of Chemical Physics</i> , 1996 , 105, 1426-1436	3.9	88
260	Wettability and friction of water on a MoS2 nanosheet. <i>Applied Physics Letters</i> , 2016 , 108, 131601	3.4	86

(2020-1995)

259	A new molecular dynamics method combining the reference system propagator algorithm with a fast multipole method for simulating proteins and other complex systems. <i>Journal of Chemical Physics</i> , 1995 , 103, 9444-9459	3.9	85	
258	Surface Curvature Relation to Protein Adsorption for Carbon-based Nanomaterials. <i>Scientific Reports</i> , 2015 , 5, 10886	4.9	84	
257	Destruction of amyloid fibrils by graphene through penetration and extraction of peptides. <i>Nanoscale</i> , 2015 , 7, 18725-37	7.7	84	
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255	Smart walking: A new method for Boltzmann sampling of protein conformations. <i>Journal of Chemical Physics</i> , 1997 , 107, 9185-9196	3.9	83	
254	Amino acid analogues bind to carbon nanotube via IIInteractions: comparison of molecular mechanical and quantum mechanical calculations. <i>Journal of Chemical Physics</i> , 2012 , 136, 025103	3.9	82	
253	The role of basic residues in the adsorption of blood proteins onto the graphene surface. <i>Scientific Reports</i> , 2015 , 5, 10873	4.9	80	
252	Cytotoxicity of graphene: recent advances and future perspective. Wiley Interdisciplinary Reviews: Nanomedicine and Nanobiotechnology, 2014 , 6, 452-74	9.2	79	
251	Nanoscale dewetting transition in protein complex folding. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 9069-77	3.4	72	
250	Hydrophobic aided replica exchange: an efficient algorithm for protein folding in explicit solvent. Journal of Physical Chemistry B, 2006 , 110, 19018-22	3.4	71	
249	How force unfolding differs from chemical denaturation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014 , 111, 3413-8	11.5	70	
248	Graphene-Induced Pore Formation on Cell Membranes. <i>Scientific Reports</i> , 2017 , 7, 42767	4.9	69	
247	A 3,2-Hydroxypyridinone-based Decorporation Agent that Removes Uranium from Bones In Vivo. <i>Nature Communications</i> , 2019 , 10, 2570	17.4	67	
246	A Peptide-Coated Gold Nanocluster Exhibits Unique Behavior in Protein Activity Inhibition. <i>Journal of the American Chemical Society</i> , 2015 , 137, 8412-8	16.4	67	
245	Hydration and dewetting near graphite-CH(3) and graphite-COOH plates. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 13639-48	3.4	67	
244	Thermal denaturing of mutant lysozyme with both the OPLSAA and the CHARMM force fields. Journal of the American Chemical Society, 2006 , 128, 13388-95	16.4	67	
243	Destruction of long-range interactions by a single mutation in lysozyme. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007 , 104, 5824-9	11.5	66	
242	Structural Basis of the Potential Binding Mechanism of Remdesivir to SARS-CoV-2 RNA-Dependent RNA Polymerase. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 6955-6962	3.4	65	

241	Drying and hydrophobic collapse of paraffin plates. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 3546-52	3.4	65
240	Hydrated Excess Protons Can Create Their Own Water Wires. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 9212-8	3.4	60
239	Single mutation induced H3N2 hemagglutinin antibody neutralization: a free energy perturbation study. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 15813-20	3.4	60
238	Hydration and dewetting near fluorinated superhydrophobic plates. <i>Journal of the American Chemical Society</i> , 2006 , 128, 12439-47	16.4	60
237	Complete wetting of graphene by biological lipids. <i>Nanoscale</i> , 2016 , 8, 5750-4	7.7	59
236	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	16.7	59
235	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, 451-63	2.8	58
234	Free energy simulations reveal a double mutant avian H5N1 virus hemagglutinin with altered receptor binding specificity. <i>Journal of Computational Chemistry</i> , 2009 , 30, 1654-63	3.5	56
233	Blue Matter, an application framework for molecular simulation on Blue Gene. <i>Journal of Parallel and Distributed Computing</i> , 2003 , 63, 759-773	4.4	56
232	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, 6826-36	16.7	55
231	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	56.2	54
230	Molecular dynamics simulations of Ago silencing complexes reveal a large repertoire of admissible 'seed-less' targets. <i>Scientific Reports</i> , 2012 , 2, 569	4.9	54
229	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, 5427-30	3.4	54
228	Palladium concave nanocrystals with high-index facets accelerate ascorbate oxidation in cancer treatment. <i>Nature Communications</i> , 2018 , 9, 4861	17.4	54
227	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	10.4	53
226	Carbon Nanotube Wins the Competitive Binding over Proline-Rich Motif Ligand on SH3 Domain. Journal of Physical Chemistry C, 2011 , 115, 12322-12328	3.8	52
225	A computationally inexpensive modification of the point dipole electrostatic polarization model for molecular simulations. <i>Journal of Computational Chemistry</i> , 2003 , 24, 267-76	3.5	51
224	Collapse of unfolded proteins in a mixture of denaturants. <i>Journal of the American Chemical Society</i> , 2012 , 134, 18266-74	16.4	50

223	High-Curvature Nanostructuring Enhances Probe Display for Biomolecular Detection. <i>Nano Letters</i> , 2017 , 17, 1289-1295	11.5	49
222	Graphene Oxide Nanosheets Retard Cellular Migration via Disruption of Actin Cytoskeleton. <i>Small</i> , 2017 , 13, 1602133	11	49
221	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; discussion e1001900	11.6	49
220	Hydrophobic interaction drives surface-assisted epitaxial assembly of amyloid-like peptides. Journal of the American Chemical Society, 2013 , 135, 3150-7	16.4	49
219	Replica exchange molecular dynamics method for protein folding simulation. <i>Methods in Molecular Biology</i> , 2007 , 350, 205-23	1.4	49
218	Urea-induced drying of hydrophobic nanotubes: comparison of different urea models. <i>Journal of Physical Chemistry B</i> , 2011 , 115, 2988-94	3.4	47
217	Molecular Dynamics with Multiple Time Scales: How to Avoid Pitfalls. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 1798-804	6.4	46
216	Membrane destruction-mediated antibacterial activity of tungsten disulfide (WS2). <i>RSC Advances</i> , 2017 , 7, 37873-37880	3.7	45
215	TcO removal from legacy defense nuclear waste by an alkaline-stable 2D cationic metal organic framework. <i>Nature Communications</i> , 2020 , 11, 5571	17.4	45
214	Nanomedicine: de novo design of nanodrugs. <i>Nanoscale</i> , 2014 , 6, 663-77	7.7	43
213	Spontaneous Transport of Single-Stranded DNA through Graphene-MoS Heterostructure Nanopores. <i>ACS Nano</i> , 2018 , 12, 3886-3891	16.7	42
212	DNA translocation through single-layer boron nitride nanopores. <i>Soft Matter</i> , 2016 , 12, 817-23	3.6	41
211	Is Poisson-Boltzmann theory insufficient for protein folding simulations?. <i>Journal of Chemical Physics</i> , 2006 , 124, 034902	3.9	40
210	Robust Antibacterial Activity of Tungsten Oxide (WO) Nanodots. <i>Chemical Research in Toxicology</i> , 2019 , 32, 1357-1366	4	39
209	Polymeric prodrugs conjugated with reduction-sensitive dextrantamptothecin and pH-responsive dextrantaxorubicin: an effective combinatorial drug delivery platform for cancer therapy. <i>Polymer Chemistry</i> , 2016 , 7, 4198-4212	4.9	39
208	Self-Assembled Core-Satellite Gold Nanoparticle Networks for Ultrasensitive Detection of Chiral Molecules by Recognition Tunneling Current. <i>ACS Nano</i> , 2016 , 10, 5096-103	16.7	39
207	Highly Sensitive Detection of UV Radiation Using a Uranium Coordination Polymer. <i>ACS Applied Materials & Acs Interfaces</i> , 2018 , 10, 4844-4850	9.5	38
206	Stability of Ligands on Nanoparticles Regulating the Integrity of Biological Membranes at the Nano-Lipid Interface. <i>ACS Nano</i> , 2019 , 13, 8680-8693	16.7	38

205	Non-destructive inhibition of metallofullerenol Gd@C(82)(OH)(22) on WW domain: implication on signal transduction pathway. <i>Scientific Reports</i> , 2012 , 2, 957	4.9	38
204	Exploration of graphene oxide as an intelligent platform for cancer vaccines. <i>Nanoscale</i> , 2015 , 7, 19949-	- 5 77	37
203	Salts drive controllable multilayered upright assembly of amyloid-like peptides at mica/water interface. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013 , 110, 8543-8	11.5	37
202	Orientational Binding of DNA Guided by the CN Template. ACS Nano, 2017, 11, 3198-3206	16.7	36
201	Structural influence of proteins upon adsorption to MoS nanomaterials: comparison of MoS force field parameters. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 3039-3045	3.6	36
200	Single-Walled Carbon Nanotubes Inhibit the Cytochrome P450 Enzyme, CYP3A4. <i>Scientific Reports</i> , 2016 , 6, 21316	4.9	36
199	A new molecular mechanism underlying the EGCG-mediated autophagic modulation of AFP in HepG2 cells. <i>Cell Death and Disease</i> , 2017 , 8, e3160	9.8	36
198	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	16.4	35
197	Exploring the Nanotoxicology of MoS: A Study on the Interaction of MoS Nanoflakes and K Channels. <i>ACS Nano</i> , 2018 , 12, 705-717	16.7	34
196	UV-radiation induced disruption of dry-cavities in human D -crystallin results in decreased stability and faster unfolding. <i>Scientific Reports</i> , 2013 , 3, 1560	4.9	33
195	Single mutation effects on conformational change and membrane deformation of influenza hemagglutinin fusion peptides. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 8799-806	3.4	33
194	Comment on "urea-mediated protein denaturation: a consensus view". <i>Journal of Physical Chemistry B</i> , 2011 , 115, 1323-6; discussion 1327-8	3.4	33
193	Simplified TiO2 force fields for studies of its interaction with biomolecules. <i>Journal of Chemical Physics</i> , 2015 , 142, 234102	3.9	32
192	Single-File Protein Translocations through Graphene-MoS Heterostructure Nanopores. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 3409-3415	6.4	32
191	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, 1446-51	3.4	32
190	Dynamics of DNA translocation in a solid-state nanopore immersed in aqueous glycerol. <i>Nanotechnology</i> , 2012 , 23, 455102	3.4	32
189	Total-energy calculations for acetylene adsorption and decomposition on Si(100)-2 x 1. <i>Physical Review B</i> , 1993 , 47, 10601-10606	3.3	32
188	Structural Damage of a Sheet Protein upon Adsorption onto Molybdenum Disulfide Nanotubes. Journal of Physical Chemistry C, 2016, 120, 6796-6803	3.8	32

(2012-2018)

187	Phase transition triggered aggregation-induced emission in a photoluminescent uranyl-organic framework. <i>Chemical Communications</i> , 2018 , 54, 627-630	5.8	31
186	Signal transmission, conversion and multiplication by polar molecules confined in nanochannels. <i>Nanoscale</i> , 2010 , 2, 1976-83	7.7	31
185	Comment on Can a Continuum Solvent Model Reproduce the Free Energy Landscape of a Hairpin Folding in Water? The Poisson Boltzmann Equation. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 7528-7530	3.4	31
184	An In Silico study of TiO nanoparticles interaction with twenty standard amino acids in aqueous solution. <i>Scientific Reports</i> , 2016 , 6, 37761	4.9	31
183	Commensal bacteria stimulate antitumor responses via T cell cross-reactivity. JCI Insight, 2020, 5,	9.9	30
182	Exploring biological effects of MoS2 nanosheets on native structures of Ehelical peptides. <i>Journal of Chemical Physics</i> , 2016 , 144, 175103	3.9	30
181	Blue Matter: Strong Scaling of Molecular Dynamics on Blue Gene/L. <i>Lecture Notes in Computer Science</i> , 2006 , 846-854	0.9	30
180	Mild Binding of Protein to C N Monolayer Reveals Its Suitable Biocompatibility. <i>Small</i> , 2017 , 13, 160368	511	28
179	beta-Strand interactions at the domain interface critical for the stability of human lens gammaD-crystallin. <i>Protein Science</i> , 2010 , 19, 131-40	6.3	28
178	Robust Denaturation of Villin Headpiece by MoS2 Nanosheet: Potential Molecular Origin of the Nanotoxicity. <i>Scientific Reports</i> , 2016 , 6, 28252	4.9	27
177	Structural and electronic properties of uranium-encapsulated Aultage. Scientific Reports, 2014, 4, 5862	4.9	26
176	Facile and Efficient Decontamination of Thorium from Rare Earths Based on Selective Selenite Crystallization. <i>Inorganic Chemistry</i> , 2018 , 57, 1880-1887	5.1	26
175	Characterization of a novel water pocket inside the human Cx26 hemichannel structure. <i>Biophysical Journal</i> , 2014 , 107, 599-612	2.9	26
174	Large scale molecular simulations of nanotoxicity. <i>Wiley Interdisciplinary Reviews: Systems Biology and Medicine</i> , 2014 , 6, 329-43	6.6	26
173	Coherent microscopic picture for urea-induced denaturation of proteins. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 8856-62	3.4	26
172	Dewetting transitions in the self-assembly of two amyloidogenic	3.4	26
171	Membrane Insertion and Phospholipids Extraction by Graphyne Nanosheets. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 2444-2450	3.8	25
170	Molecular mechanism of surface-assisted epitaxial self-assembly of amyloid-like peptides. <i>ACS Nano</i> , 2012 , 6, 9276-82	16.7	25

169	The folding transition state of protein L is extensive with nonnative interactions (and not small and polarized). <i>Journal of Molecular Biology</i> , 2012 , 420, 220-34	6.5	25
168	Using a mutual information-based site transition network to map the genetic evolution of influenza A/H3N2 virus. <i>Bioinformatics</i> , 2009 , 25, 2309-17	7.2	25
167	Stimulating antibacterial activities of graphitic carbon nitride nanosheets with plasma treatment. <i>Nanoscale</i> , 2019 , 11, 18416-18425	7.7	24
166	Impacts of fullerene derivatives on regulating the structure and assembly of collagen molecules. <i>Nanoscale</i> , 2013 , 5, 7341-8	7.7	24
165	Molecular Structure and Dynamics of Water on Pristine and Strained Phosphorene: Wetting and Diffusion at Nanoscale. <i>Scientific Reports</i> , 2016 , 6, 38327	4.9	24
164	Successful Decontamination of 99TcO4lin Groundwater at Legacy Nuclear Sites by a Cationic Metal-Organic Framework with Hydrophobic Pockets. <i>Angewandte Chemie</i> , 2019 , 131, 5022-5026	3.6	24
163	Emerging Sheet Rich Conformations in Supercompact Huntingtin Exon-1 Mutant Structures. Journal of the American Chemical Society, 2017 , 139, 8820-8827	16.4	23
162	Hydrogen and methane storage and release by MoS2 nanotubes for energy storage. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 23020-23027	13	23
161	Defect-assisted protein HP35 denaturation on graphene. <i>Nanoscale</i> , 2019 , 11, 19362-19369	7.7	23
160	Lanosterol Disrupts Aggregation of Human D -Crystallin by Binding to the Hydrophobic Dimerization Interface. <i>Journal of the American Chemical Society</i> , 2018 , 140, 8479-8486	16.4	23
159	Multiscale modeling of macromolecular biosystems. <i>Briefings in Bioinformatics</i> , 2012 , 13, 395-405	13.4	23
158	Emergence of a Radical-Stabilizing Metal-Organic Framework as a Radio-photoluminescence Dosimeter. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 15209-15214	16.4	22
157	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	11.5	22
156	Thickness dependent semiconductor-to-metal transition of two-dimensional polyaniline with unique work functions. <i>Nanoscale</i> , 2017 , 9, 12025-12031	7.7	22
155	Enantiomerization mechanism of thalidomide and the role of water and hydroxide ions. <i>Chemistry - A European Journal</i> , 2012 , 18, 14305-13	4.8	22
154	Free-energy simulations reveal that both hydrophobic and polar interactions are important for influenza hemagglutinin antibody binding. <i>Biophysical Journal</i> , 2012 , 102, 1453-61	2.9	22
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(2020-2016)

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LIST OF PUBLICATIONS

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