

Ruhong Zhou

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

312
papers

18,147
citations

67
h-index

126
g-index

338
ext. papers

20,858
ext. citations

8.1
avg, IF

7
L-index

#	Paper	IF	Citations
312	Graphene oxide toxicity in W flies. <i>Science of the Total Environment</i> , 2022 , 805, 150302	10.2	3
311	Role of polyplex charge density in lipopolyplexes.. <i>Nanoscale</i> , 2022 , 14, 7174-7180	7.7	
310	Distinct lipid membrane interaction and uptake of differentially charged nanoplastics in bacteria.. <i>Journal of Nanobiotechnology</i> , 2022 , 20, 191	9.4	1
309	Potential interference of graphene nanosheets in immune response disrupting the recognition of HLA-presented KK10 by TCR: a molecular dynamics simulation study. <i>Nanoscale</i> , 2021 , 13, 19255-19263	7.7	1
308	Modeling Noncanonical RNA Base Pairs by a Coarse-Grained IsRNA2 Model. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 11907-11915	3.4	1
307	Molecular Insight into AC Electric Field Enhanced Removal of Protein Aggregates from a Material Surface. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 12147-12153	3.4	
306	Molecular Dynamics Simulation Study on Interactions of Cycloviolacin with Different Phospholipids. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 3476-3485	3.4	2
305	Biotransformation of rare earth oxide nanoparticles eliciting microbiota imbalance. <i>Particle and Fibre Toxicology</i> , 2021 , 18, 17	8.4	1
304	Dose-Independent Transfection of Hydrophobized Polyplexes. <i>Advanced Materials</i> , 2021 , 33, e2102219	24	6
303	Multifaceted Regulation of Potassium-Ion Channels by Graphene Quantum Dots. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 27784-27795	9.5	1
302	CASTELO: clustered atom subtypes aided lead optimization-a combined machine learning and molecular modeling method. <i>BMC Bioinformatics</i> , 2021 , 22, 338	3.6	0
301	Ionic conductance oscillations in sub-nanometer pores probed by optoelectronic control. <i>Matter</i> , 2021 , 4, 2378-2391	12.7	2
300	Metallo-Helicoid with Double Rims: Polymerization Followed by Folding by Intramolecular Coordination. <i>Angewandte Chemie</i> , 2021 , 133, 1301-1309	3.6	1
299	Metallo-Helicoid with Double Rims: Polymerization Followed by Folding by Intramolecular Coordination. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 1281-1289	16.4	6
298	Dioxybenzone triggers enhanced estrogenic effect via metabolic activation: in silico, in vitro and in vivo investigation. <i>Environmental Pollution</i> , 2021 , 268, 115766	9.3	4
297	Molecular mechanism of secreted amyloid- β precursor protein in binding and modulating GABAR1a. <i>Chemical Science</i> , 2021 , 12, 6107-6116	9.4	2
296	Self-cascade MoS nanozymes for efficient intracellular antioxidation and hepatic fibrosis therapy. <i>Nanoscale</i> , 2021 , 13, 12613-12622	7.7	4

295	Boron nitride nanosheets elicit significant hemolytic activity via destruction of red blood cell membranes. <i>Colloids and Surfaces B: Biointerfaces</i> , 2021 , 203, 111765	6	5
294	Hydrophobic collapse-driven nanoparticle coating with poly-adenine adhesives. <i>Chemical Communications</i> , 2021 , 57, 3801-3804	5.8	5
293	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
292	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
291	Planar graphene/h-BN/graphene heterostructures for protein stretching and confinement. <i>Nanoscale</i> , 2020 , 12, 13822-13828	7.7	6
290	Tungsten Oxide Nanodots Exhibit Mild Interactions with WW and SH3 Modular Protein Domains. <i>ACS Omega</i> , 2020 , 5, 11005-11012	3.9	0
289	A Porous Aromatic Framework Functionalized with Luminescent Iridium(III) Organometallic Complexes for Turn-On Sensing of TcO. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 15288-15297	9.5	17
288	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
287	Graphene-extracted membrane lipids facilitate the activation of integrin β . <i>Nanoscale</i> , 2020 , 12, 7939-7949	7.7	11
286	Half a century of amyloids: past, present and future. <i>Chemical Society Reviews</i> , 2020 , 49, 5473-5509	58.5	142
285	Stabilization of Open-Shell Single Bonds within Endohedral Metallofullerene. <i>Inorganic Chemistry</i> , 2020 , 59, 3606-3618	5.1	6
284	Directional extraction and penetration of phosphorene nanosheets to cell membranes. <i>Nanoscale</i> , 2020 , 12, 2810-2819	7.7	11
283	Retained Stability of the RNA Structure in DNA Packaging Motor with a Single Mg Ion Bound at the Double Mg-Clamp Structure. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 701-707	3.4	2
282	N-Oxide polymer-cupric ion nanogels potentiate disulfiram for cancer therapy. <i>Biomaterials Science</i> , 2020 , 8, 1726-1733	7.4	5
281	Zipper-Like Unfolding of dsDNA Caused by Graphene Wrinkles. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 3332-3340	3.8	6
280	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
279	Binding patterns and dynamics of double-stranded DNA on the phosphorene surface. <i>Nanoscale</i> , 2020 , 12, 9430-9439	7.7	11
278	Commensal bacteria stimulate antitumor responses via T cell cross-reactivity. <i>JCI Insight</i> , 2020 , 5,	9.9	30

277	Proteasome activity regulated by charged gold nanoclusters: Implications for neurodegenerative diseases. <i>Nano Today</i> , 2020 , 35, 100933	17.9	3
276	HIV-1 induced changes in HLA-C*03 : 04-presented peptide repertoires lead to reduced engagement of inhibitory natural killer cell receptors. <i>Aids</i> , 2020 , 34, 1713-1723	3.5	6
275	Spontaneous Translocation of Single-Stranded DNA in Graphene-MoS Heterostructure Nanopores: Shape Effect. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 9490-9496	3.4	4
274	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
273	Low-Dose X-ray-Responsive Diselenide Nanocarriers for Effective Delivery of Anticancer Agents. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 43398-43407	9.5	10
272	Partial Denaturation of Villin Headpiece upon Binding to a Carbon Nitride Polyaniline (CN) Nanosheet. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 7557-7563	3.4	4
271	Emergence of a Radical-Stabilizing Metal-Organic Framework as a Radio-photoluminescence Dosimeter. <i>Angewandte Chemie</i> , 2020 , 132, 15321-15326	3.6	4
270	Stimulating antibacterial activities of graphitic carbon nitride nanosheets with plasma treatment. <i>Nanoscale</i> , 2019 , 11, 18416-18425	7.7	24
269	Different platinum crystal surfaces show very distinct protein denaturation capabilities. <i>Nanoscale</i> , 2019 , 11, 19352-19361	7.7	3
268	Modeling and Structural Characterization of the Sweet Taste Receptor Heterodimer. <i>ACS Chemical Neuroscience</i> , 2019 , 10, 4579-4592	5.7	10
267	Facet-regulated adhesion of double-stranded DNA on palladium surfaces. <i>Nanoscale</i> , 2019 , 11, 1827-1836	7.7	9
266	Inorganic X-ray Scintillators Based on a Previously Unnoticed but Intrinsically Advantageous Metal Center. <i>Inorganic Chemistry</i> , 2019 , 58, 2807-2812	5.1	7
265	Robust Antibacterial Activity of Tungsten Oxide (WO) Nanodots. <i>Chemical Research in Toxicology</i> , 2019 , 32, 1357-1366	4	39
264	A 3,2-Hydroxypyridinone-based Decorporation Agent that Removes Uranium from Bones In Vivo. <i>Nature Communications</i> , 2019 , 10, 2570	17.4	67
263	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
262	Different protonated states at the C-terminal of the amyloid- β peptide modulate the stability of S-shaped protofibril. <i>Journal of Chemical Physics</i> , 2019 , 150, 185102	3.9	3
261	Molecular Origin of the Stability Difference in Four Shark IgNAR Constant Domains. <i>Biophysical Journal</i> , 2019 , 116, 1907-1917	2.9	2
260	Defect-assisted protein HP35 denaturation on graphene. <i>Nanoscale</i> , 2019 , 11, 19362-19369	7.7	23

259	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	16.4	16
258	Protein WW domain denaturation on defective graphene reveals the significance of nanomaterial defects in nanotoxicity. <i>Carbon</i> , 2019 , 146, 257-264	10.4	19
257	Exploration of HIV-1 fusion peptide-antibody VRC34.01 binding reveals fundamental neutralization sites. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 18569-18576	3.6	3
256	Lanosterol Disrupts the Aggregation of Amyloid- β Peptides. <i>ACS Chemical Neuroscience</i> , 2019 , 10, 4051-4060	9.6	7
255	Parameterization of Molybdenum Disulfide Interacting with Water Using the Free Energy Perturbation Method. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 7243-7252	3.4	3
254	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
253	Surface Inhomogeneity of Graphene Oxide Influences Dissociation of A β Peptide Assembly. <i>Journal of Physical Chemistry B</i> , 2019 , 123, 9098-9103	3.4	10
252	Spontaneous ssDNA stretching on graphene and hexagonal boron nitride in plane heterostructures. <i>Nature Communications</i> , 2019 , 10, 4610	17.4	17
251	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
250	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
249	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	3.6	24
248	The molecular mechanism of robust macrophage immune responses induced by PEGylated molybdenum disulfide. <i>Nanoscale</i> , 2019 , 11, 22293-22304	7.7	18
247	Physical and Toxicological Profiles of Human IAPP Amyloids and Plaques. <i>Science Bulletin</i> , 2019 , 64, 26-35	10.6	15
246	Atomic-Scale Fluidic Diodes Based on Triangular Nanopores in Bilayer Hexagonal Boron Nitride. <i>Nano Letters</i> , 2019 , 19, 977-982	11.5	22
245	Exploring the binding mechanism between human profilin (PFN1) and polyproline-10 through binding mode screening. <i>Journal of Chemical Physics</i> , 2019 , 150, 015102	3.9	1
244	Charging nanoparticles: increased binding of Gd@C(OH) derivatives to human MMP-9. <i>Nanoscale</i> , 2018 , 10, 5667-5677	7.7	17
243	COR+ (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	13	18
242	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

241	Rare Dissipative Transitions Punctuate the Initiation of Chemical Denaturation in Proteins. <i>Biophysical Journal</i> , 2018 , 114, 812-821	2.9	
240	Spontaneous Transport of Single-Stranded DNA through Graphene-MoS Heterostructure Nanopores. <i>ACS Nano</i> , 2018 , 12, 3886-3891	16.7	42
239	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
238	Inhibition of the proteasome activity by graphene oxide contributes to its cytotoxicity. <i>Nanotoxicology</i> , 2018 , 12, 185-200	5.3	13
237	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	11.5	10
236	Inhibition of CYP2C8 by metallofullerenol Gd@C82(OH)22 through blocking substrate channels and substrate recognition sites. <i>Carbon</i> , 2018 , 127, 667-675	10.4	8
235	Phase transition triggered aggregation-induced emission in a photoluminescent uranyl-organic framework. <i>Chemical Communications</i> , 2018 , 54, 627-630	5.8	31
234	Binding Specificity Determines the Cytochrome P450 3A4 Mediated Enantioselective Metabolism of Metconazole. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 1176-1184	3.4	21
233	Highly Sensitive Detection of UV Radiation Using a Uranium Coordination Polymer. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 4844-4850	9.5	38
232	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
231	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	5.1	6
230	Mechanism by which DHA inhibits the aggregation of KLVFFA peptides: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 2018 , 148, 115102	3.9	7
229	Molecular mechanism of Gd@C(OH) increasing collagen expression: Implication for engaging tumor. <i>Biomaterials</i> , 2018 , 152, 24-36	15.6	20
228	Degradable Carbon Dots with Broad-Spectrum Antibacterial Activity. <i>ACS Applied Materials & Interfaces</i> , 2018 , 10, 26936-26946	9.5	143
227	Glassy dynamics in mutant huntingtin proteins. <i>Journal of Chemical Physics</i> , 2018 , 149, 072333	3.9	4
226	Single-File Protein Translocations through Graphene-MoS Heterostructure Nanopores. <i>Journal of Physical Chemistry Letters</i> , 2018 , 9, 3409-3415	6.4	32
225	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
224	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

223	Patient HLA class I genotype influences cancer response to checkpoint blockade immunotherapy. <i>Science</i> , 2018 , 359, 582-587	33.3	500
222	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	3.6	13
221	Palladium concave nanocrystals with high-index facets accelerate ascorbate oxidation in cancer treatment. <i>Nature Communications</i> , 2018 , 9, 4861	17.4	54
220	Superior Compatibility of C N with Human Red Blood Cell Membranes and the Underlying Mechanism. <i>Small</i> , 2018 , 14, e1803509	11	20
219	Molecular mechanism of phosphoinositides' specificity for the inwardly rectifying potassium channel Kir2.2. <i>Chemical Science</i> , 2018 , 9, 8352-8362	9.4	0
218	Membrane Insertion and Phospholipids Extraction by Graphyne Nanosheets. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 2444-2450	3.8	25
217	High-Curvature Nanostructuring Enhances Probe Display for Biomolecular Detection. <i>Nano Letters</i> , 2017 , 17, 1289-1295	11.5	49
216	Mild Binding of Protein to C N Monolayer Reveals Its Suitable Biocompatibility. <i>Small</i> , 2017 , 13, 160368511		28
215	Graphene-Induced Pore Formation on Cell Membranes. <i>Scientific Reports</i> , 2017 , 7, 42767	4.9	69
214	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	10.3	246
213	PEGylated graphene oxide elicits strong immunological responses despite surface passivation. <i>Nature Communications</i> , 2017 , 8, 14537	17.4	120
212	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	3.4	9
211	A novel self-activation mechanism of <i>Candida antarctica</i> lipase B. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 15709-15714	3.6	8
210	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
209	Overcoming the crystallization and designability issues in the ultrastable zirconium phosphonate framework system. <i>Nature Communications</i> , 2017 , 8, 15369	17.4	266
208	Understanding the graphene quantum dots-ubiquitin interaction by identifying the interaction sites. <i>Carbon</i> , 2017 , 121, 285-291	10.4	13
207	Emerging Sheet Rich Conformations in Supercompact Huntingtin Exon-1 Mutant Structures. <i>Journal of the American Chemical Society</i> , 2017 , 139, 8820-8827	16.4	23
206	Impact of graphyne on structural and dynamical properties of calmodulin. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 10187-10195	3.6	8

205	Orientational Binding of DNA Guided by the CN Template. <i>ACS Nano</i> , 2017 , 11, 3198-3206	16.7	36
204	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
203	Snatching the Ligand or Destroying the Structure: Disruption of WW Domain by Phosphorene. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 1362-1370	3.8	10
202	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
201	Hydrogen and methane storage and release by MoS ₂ nanotubes for energy storage. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 23020-23027	13	23
200	Phosphatidylserine-Induced Conformational Modulation of Immune Cell Exhaustion-Associated Receptor TIM3. <i>Scientific Reports</i> , 2017 , 7, 13579	4.9	3
199	Directional mechanical stability of Bacteriophage ϕ 9 motor's 3WJ-pRNA: Extraordinary robustness along portal axis. <i>Science Advances</i> , 2017 , 3, e1601684	14.3	14
198	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
197	Humidity-Responsive Single-Nanoparticle-Layer Plasmonic Films. <i>Advanced Materials</i> , 2017 , 29, 160679624		21
196	Thickness dependent semiconductor-to-metal transition of two-dimensional polyaniline with unique work functions. <i>Nanoscale</i> , 2017 , 9, 12025-12031	7.7	22
195	Structural perturbations on huntingtin N17 domain during its folding on 2D-nanomaterials. <i>Nanotechnology</i> , 2017 , 28, 354001	3.4	8
194	Membrane destruction-mediated antibacterial activity of tungsten disulfide (WS ₂). <i>RSC Advances</i> , 2017 , 7, 37873-37880	3.7	45
193	Detecting Interactions between Nanomaterials and Cell Membranes by Synthetic Nanopores. <i>ACS Nano</i> , 2017 , 11, 12615-12623	16.7	18
192	A mesoporous cationic thorium-organic framework that rapidly traps anionic persistent organic pollutants. <i>Nature Communications</i> , 2017 , 8, 1354	17.4	211
191	Graphene Oxide Nanosheets Retard Cellular Migration via Disruption of Actin Cytoskeleton. <i>Small</i> , 2017 , 13, 1602133	11	49
190	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	3.9	2
189	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
188	Concentration-dependent binding of CdSe quantum dots on the SH3 domain. <i>Nanoscale</i> , 2017 , 10, 351-358		4

187	The Molecular Mechanism of Opening the Helix Bundle Crossing (HBC) Gate of a Kir Channel. <i>Scientific Reports</i> , 2016 , 6, 29399	4.9	17
186	Robust Denaturation of Villin Headpiece by MoS ₂ Nanosheet: Potential Molecular Origin of the Nanotoxicity. <i>Scientific Reports</i> , 2016 , 6, 28252	4.9	27
185	Single-Walled Carbon Nanotubes Inhibit the Cytochrome P450 Enzyme, CYP3A4. <i>Scientific Reports</i> , 2016 , 6, 21316	4.9	36
184	Folding and Stabilization of Native-Sequence-Reversed Proteins. <i>Scientific Reports</i> , 2016 , 6, 25138	4.9	3
183	Mechanism of Divalent-Ion-Induced Charge Inversion of Bacterial Membranes. <i>Journal of Physical Chemistry Letters</i> , 2016 , 7, 2434-8	6.4	15
182	Exploring the Membrane Potential of Simple Dual-Membrane Systems as Models for Gap-Junction Channels. <i>Biophysical Journal</i> , 2016 , 110, 2678-2688	2.9	8
181	Opening Lids: Modulation of Lipase Immobilization by Graphene Oxides. <i>ACS Catalysis</i> , 2016 , 6, 4760-4768	6.1	103
180	Tunable, Strain-Controlled Nanoporous MoS ₂ Filter for Water Desalination. <i>ACS Nano</i> , 2016 , 10, 1829-35	16.7	174
179	Sequential protein unfolding through a carbon nanotube pore. <i>Nanoscale</i> , 2016 , 8, 12143-51	7.7	12
178	Complete wetting of graphene by biological lipids. <i>Nanoscale</i> , 2016 , 8, 5750-4	7.7	59
177	Potential Interference of Protein-Protein Interactions by Graphyne. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 2124-31	3.4	13
176	Toward high permeability, selectivity and controllability of water desalination with FePc nanopores. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 8140-7	3.6	10
175	Nanomechanics of Protein Unfolding Outside a Generic Nanopore. <i>ACS Nano</i> , 2016 , 10, 317-23	16.7	20
174	DNA translocation through single-layer boron nitride nanopores. <i>Soft Matter</i> , 2016 , 12, 817-23	3.6	41
173	An In Silico study of TiO ₂ nanoparticles interaction with twenty standard amino acids in aqueous solution. <i>Scientific Reports</i> , 2016 , 6, 37761	4.9	31
172	EGCG in Green Tea Induces Aggregation of HMGB1 Protein through Large Conformational Changes with Polarized Charge Redistribution. <i>Scientific Reports</i> , 2016 , 6, 22128	4.9	13
171	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
170	Potential disruption of protein-protein interactions by graphene oxide. <i>Journal of Chemical Physics</i> , 2016 , 144, 225102	3.9	17

169	Exploring biological effects of MoS ₂ nanosheets on native structures of α -helical peptides. <i>Journal of Chemical Physics</i> , 2016 , 144, 175103	3.9	30
168	Wettability and friction of water on a MoS ₂ nanosheet. <i>Applied Physics Letters</i> , 2016 , 108, 131601	3.4	86
167	Structural Damage of a Sheet Protein upon Adsorption onto Molybdenum Disulfide Nanotubes. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 6796-6803	3.8	32
166	Polymeric prodrugs conjugated with reduction-sensitive dextran- α -amptothecin and pH-responsive dextran- α -doxorubicin: an effective combinatorial drug delivery platform for cancer therapy. <i>Polymer Chemistry</i> , 2016 , 7, 4198-4212	4.9	39
165	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
164	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
163	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, 8302-7	11.5	17
162	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
161	Simplified TiO ₂ force fields for studies of its interaction with biomolecules. <i>Journal of Chemical Physics</i> , 2015 , 142, 234102	3.9	32
160	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
159	Surface Curvature Relation to Protein Adsorption for Carbon-based Nanomaterials. <i>Scientific Reports</i> , 2015 , 5, 10886	4.9	84
158	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
157	Water film inside graphene nanosheets: electron transfer reversal between water and graphene via tight nano-confinement. <i>RSC Advances</i> , 2015 , 5, 274-280	3.7	17
156	Modeling of Nanotoxicity 2015 ,		10
155	Quantum Dots and Their Ligand Passivation 2015 , 131-145		
154	Exploration of graphene oxide as an intelligent platform for cancer vaccines. <i>Nanoscale</i> , 2015 , 7, 19949-57		37
153	Destruction of amyloid fibrils by graphene through penetration and extraction of peptides. <i>Nanoscale</i> , 2015 , 7, 18725-37	7.7	84
152	Nanomedicine: Implications from Nanotoxicity 2015 , 147-168		

151 Graphene and Derivatives **2015**, 61-88

150 Fullerene and Derivatives **2015**, 17-43

149 Protein corona mitigates the cytotoxicity of graphene oxide by reducing its physical interaction with cell membrane. *Nanoscale*, **2015**, 7, 15214-24 7.7 157

148 A novel form of β -strand assembly observed in A β (33-42) adsorbed onto graphene. *Nanoscale*, **2015**, 7, 15341-8 7.7 19

147 Potential toxicity of graphene to cell functions via disrupting protein-protein interactions. *ACS Nano*, **2015**, 9, 663-9 16.7 143

146 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; discussion e1001900 11.6 49

145 Reduced Cytotoxicity of Graphene Nanosheets Mediated by Blood-Protein Coating. *ACS Nano*, **2015**, 9, 5713-24 16.7 216

144 Ionic liquid induced inactivation of cellobiohydrolase I from *Trichoderma reesei*. *Green Chemistry*, **2015**, 17, 1618-1625 10 18

143 Hydrated Excess Protons Can Create Their Own Water Wires. *Journal of Physical Chemistry B*, **2015**, 119, 9212-8 3.4 60

142 Towards understanding of nanoparticle-protein corona. *Archives of Toxicology*, **2015**, 89, 519-39 5.8 112

141 Nanopore-Based Sensors for Ligand-Receptor Lead Optimization. *Journal of Physical Chemistry Letters*, **2015**, 6, 331-7 6.4 5

140 Graphyne and Derivatives **2015**, 89-100

139 Noble Metal Nanomaterials **2015**, 101-113

138 Metal Oxides and Related Nanostructures **2015**, 115-130 0

137 Dual inhibitory pathways of metallofullerenol Gd@C₇₀(OH)₁₂ on matrix metalloproteinase-2: molecular insight into drug-like nanomedicine. *Scientific Reports*, **2014**, 4, 4775 4.9 19

136 Structural and electronic properties of uranium-encapsulated Au cage. *Scientific Reports*, **2014**, 4, 5862 4.9 26

135 Rotation motion of designed nano-turbine. *Scientific Reports*, **2014**, 4, 5846 4.9 20

134 How force unfolding differs from chemical denaturation. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 3413-8 11.5 70

133	Conformation-dependent DNA attraction. <i>Nanoscale</i> , 2014 , 6, 7085-92	7.7	11
132	Molecular recognition of metabotropic glutamate receptor type 1 (mGluR1): synergistic understanding with free energy perturbation and linear response modeling. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 6393-404	3.4	2
131	Nanomedicine: de novo design of nanodrugs. <i>Nanoscale</i> , 2014 , 6, 663-77	7.7	43
130	Irreversible denaturation of proteins through aluminum-induced formation of backbone ring structures. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 6358-63	16.4	16
129	Effect of ligands on the characteristics of (CdSe) ₁₃ quantum dots. <i>RSC Advances</i> , 2014 , 4, 27146-27151	3.7	19
128	Dissecting the contributions of hairpin tyrosine pairs to the folding and stability of long-lived human D-crystallins. <i>Nanoscale</i> , 2014 , 6, 1797-807	7.7	7
127	Cytotoxicity of graphene: recent advances and future perspective. <i>Wiley Interdisciplinary Reviews: Nanomedicine and Nanobiotechnology</i> , 2014 , 6, 452-74	9.2	79
126	Effect of urea concentration on aggregation of amyloidogenic hexapeptides (NFGAIL). <i>Journal of Physical Chemistry B</i> , 2014 , 118, 48-57	3.4	14
125	Characterization of a novel water pocket inside the human Cx26 hemichannel structure. <i>Biophysical Journal</i> , 2014 , 107, 599-612	2.9	26
124	An improved DNA force field for ssDNA interactions with gold nanoparticles. <i>Journal of Chemical Physics</i> , 2014 , 140, 234102	3.9	10
123	Controlled transport of DNA through a Y-shaped carbon nanotube in a solid membrane. <i>Nanoscale</i> , 2014 , 6, 11479-83	7.7	11
122	Carbon nanotubes adsorb U atoms differently in their inner and outer surfaces. <i>RSC Advances</i> , 2014 , 4, 30074	3.7	10
121	Path Integral Coarse-Graining Replica Exchange Method for Enhanced Sampling. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 3634-40	6.4	9
120	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, 2800-11	7.7	83
119	Size-dependent impact of CNTs on dynamic properties of calmodulin. <i>Nanoscale</i> , 2014 , 6, 12828-37	7.7	15
118	Large scale molecular simulations of nanotoxicity. <i>Wiley Interdisciplinary Reviews: Systems Biology and Medicine</i> , 2014 , 6, 329-43	6.6	26
117	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	4.9	16
116	Bio-mimicking of proline-rich motif applied to carbon nanotube reveals unexpected subtleties underlying nanoparticle functionalization. <i>Scientific Reports</i> , 2014 , 4, 7229	4.9	4

115	Dewetting transition assisted clearance of (NFGAILS) amyloid fibrils from cell membranes by graphene. <i>Journal of Chemical Physics</i> , 2014 , 141, 22D520	3.9	12
114	The ground state and electronic structure of Gd@C82: a systematic theoretical investigation of first principle density functionals. <i>Journal of Chemical Physics</i> , 2014 , 141, 244306	3.9	20
113	A unique feature of chiral transition of a difluorobenzo[c]phenanthrene molecule confined in a boron-nitride nanotube based on molecular dynamics simulations. <i>Chemical Physics Letters</i> , 2014 , 591, 265-267	2.5	5
112	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, 3541-7	3.4	12
111	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	3.9	17
110	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
109	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	3.9	11
108	Metallofullerenol Gd@C(OH) _n distracts the proline-rich-motif from putative binding on the SH3 domain. <i>Nanoscale</i> , 2013 , 5, 2703-12	7.7	21
107	Small Molecules and Peptides Inside Carbon Nanotubes: Impact of Nanoscale Confinement 2013 ,		2
106	Ethanol promotes dewetting transition at low concentrations. <i>Soft Matter</i> , 2013 , 9, 4655	3.6	17
105	Hydrophobic interaction drives surface-assisted epitaxial assembly of amyloid-like peptides. <i>Journal of the American Chemical Society</i> , 2013 , 135, 3150-7	16.4	49
104	Impacts of fullerene derivatives on regulating the structure and assembly of collagen molecules. <i>Nanoscale</i> , 2013 , 5, 7341-8	7.7	24
103	Destructive extraction of phospholipids from Escherichia coli membranes by graphene nanosheets. <i>Nature Nanotechnology</i> , 2013 , 8, 594-601	28.7	1008
102	Interplay between drying and stability of a TIM barrel protein: a combined simulation-experimental study. <i>Journal of the American Chemical Society</i> , 2013 , 135, 1882-90	16.4	20
101	Collapse of a hydrophobic polymer in a mixture of denaturants. <i>Langmuir</i> , 2013 , 29, 4877-82	4	18
100	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
99	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
98	Large domain motions in Ago protein controlled by the guide DNA-strand seed region determine the Ago-DNA-mRNA complex recognition process. <i>PLoS ONE</i> , 2013 , 8, e54620	3.7	12

97	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
96	Molecular wire of urea in carbon nanotube: a molecular dynamics study. <i>Nanoscale</i> , 2012 , 4, 652-8	7.7	18
95	Probing the self-assembly mechanism of diphenylalanine-based peptide nanovesicles and nanotubes. <i>ACS Nano</i> , 2012 , 6, 3907-18	16.7	213
94	How does water-nanotube interaction influence water flow through the nanochannel?. <i>Journal of Chemical Physics</i> , 2012 , 136, 175101	3.9	14
93	Nanopore-Based Sensors for Detecting Toxicity of a Carbon Nanotube to Proteins. <i>Journal of Physical Chemistry Letters</i> , 2012 , 2012, 2337-2341	6.4	16
92	Molecular mechanism of surface-assisted epitaxial self-assembly of amyloid-like peptides. <i>ACS Nano</i> , 2012 , 6, 9276-82	16.7	25
91	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
90	Collapse of unfolded proteins in a mixture of denaturants. <i>Journal of the American Chemical Society</i> , 2012 , 134, 18266-74	16.4	50
89	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
88	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
87	Novel Design of a Nanoflowmeter Based on Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 13429-13434	3.8	6
86	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
85	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	0.5	6
84	Amino acid analogues bind to carbon nanotube via π -interactions: comparison of molecular mechanical and quantum mechanical calculations. <i>Journal of Chemical Physics</i> , 2012 , 136, 025103	3.9	82
83	Coherent microscopic picture for urea-induced denaturation of proteins. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 8856-62	3.4	26
82	Comprehensive interrogation of natural TALE DNA-binding modules and transcriptional repressor domains. <i>Nature Communications</i> , 2012 , 3, 968	17.4	257
81	Multiscale modeling of macromolecular biosystems. <i>Briefings in Bioinformatics</i> , 2012 , 13, 395-405	13.4	23
80	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

79	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
78	Dynamics of DNA translocation in a solid-state nanopore immersed in aqueous glycerol. <i>Nanotechnology</i> , 2012 , 23, 455102	3.4	32
77	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, 10514-9	11.5	100
76	Nanotoxicity: Exploring the Interactions Between Carbon Nanotubes and Proteins 2011 ,		1
75	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
74	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
73	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	3.8	52
72	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
71	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
70	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, 11137-44	3.4	26
69	Plugging into proteins: poisoning protein function by a hydrophobic nanoparticle. <i>ACS Nano</i> , 2010 , 4, 7508-14	16.7	155
68	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
67	Key residues that play a critical role in urea-induced lysozyme unfolding. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 15687-93	3.4	17
66	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
65	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
64	Signal transmission, conversion and multiplication by polar molecules confined in nanochannels. <i>Nanoscale</i> , 2010 , 2, 1976-83	7.7	31
63	β -strand interactions at the domain interface critical for the stability of human lens γ -D-crystallin. <i>Protein Science</i> , 2010 , 19, 131-40	6.3	28
62	Size dependence of nanoscale confinement on chiral transformation. <i>Chemistry - A European Journal</i> , 2010 , 16, 6482-7	4.8	5

61	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
60	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	2	4
59	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
58	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
57	Dewetting and hydrophobic interaction in physical and biological systems. <i>Annual Review of Physical Chemistry</i> , 2009 , 60, 85-103	15.7	383
56	Recognition mechanism of siRNA by viral p19 suppressor of RNA silencing: a molecular dynamics study. <i>Biophysical Journal</i> , 2009 , 96, 1761-9	2.9	17
55	Urea's action on hydrophobic interactions. <i>Journal of the American Chemical Society</i> , 2009 , 131, 1535-41	16.4	261
54	Role of water in mediating the assembly of Alzheimer amyloid-beta Abeta16-22 protofilaments. <i>Journal of the American Chemical Society</i> , 2008 , 130, 11066-72	16.4	180
53	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
52	Sequence-based protein domain boundary prediction using BP neural network with various property profiles. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008 , 71, 300-7	4.2	8
51	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
50	Nanoscale dewetting transition in protein complex folding. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 9069-77	3.4	72
49	Replica exchange with solute tempering: efficiency in large scale systems. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 5405-10	3.4	95
48	Replica exchange molecular dynamics method for protein folding simulation. <i>Methods in Molecular Biology</i> , 2007 , 350, 205-23	1.4	49
47	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
46	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
45	PROTERAN: animated terrain evolution for visual analysis of patterns in protein folding trajectory. <i>Bioinformatics</i> , 2007 , 23, 99-106	7.2	13
44	Single-mutation-induced stability loss in protein lysozyme. <i>Biochemical Society Transactions</i> , 2007 , 35, 1551-7	5.1	11

43	Is Poisson-Boltzmann theory insufficient for protein folding simulations?. <i>Journal of Chemical Physics</i> , 2006 , 124, 034902	3.9	40
42	A combined steepest descent and genetic algorithm (SD/GA) approach for the optimization of solvation parameters. <i>Molecular Simulation</i> , 2006 , 32, 427-435	2	2
41	Thermal denaturing of mutant lysozyme with both the OPLSAA and the CHARMM force fields. <i>Journal of the American Chemical Society</i> , 2006 , 128, 13388-95	16.4	67
40	Hydrophobic aided replica exchange: an efficient algorithm for protein folding in explicit solvent. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 19018-22	3.4	71
39	Hydration and dewetting near fluorinated superhydrophobic plates. <i>Journal of the American Chemical Society</i> , 2006 , 128, 12439-47	16.4	60
38	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
37	Magnitude and spatial orientation of the hydrophobic moments of multi-domain proteins. <i>International Journal of Bioinformatics Research and Applications</i> , 2006 , 2, 161-76	0.9	2
36	Blue Matter: Strong Scaling of Molecular Dynamics on Blue Gene/L. <i>Lecture Notes in Computer Science</i> , 2006 , 846-854	0.9	30
35	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
34	Drying and hydrophobic collapse of paraffin plates. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 3546-52	3.4	65
33	A wavelet approach for the analysis of folding trajectory of protein Trp-cage. <i>Journal of Bioinformatics and Computational Biology</i> , 2005 , 3, 1351-70	1	6
32	Protein Folding with the Parallel Replica Exchange Molecular Dynamics Method 2005 , 395-425		
31	Observation of a dewetting transition in the collapse of the melittin tetramer. <i>Nature</i> , 2005 , 437, 159-62	50.4	333
30	Combinatorial pattern discovery approach for the folding trajectory analysis of a beta-hairpin. <i>PLoS Computational Biology</i> , 2005 , 1, e8	5	4
29	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
28	Hydrophobic collapse in multidomain protein folding. <i>Science</i> , 2004 , 305, 1605-9	33.3	441
27	Comment on "Can a Continuum Solvent Model Reproduce the Free Energy Landscape of a β -Hairpin Folding in Water?" The Poisson-Boltzmann Equation. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 7528-7530	3.4	31
26	Describing Protein Folding Kinetics by Molecular Dynamics Simulations. 2. Example Applications to Alanine Dipeptide and a β -Hairpin Peptide <i>Journal of Physical Chemistry B</i> , 2004 , 108, 6582-6594	3.4	159

25	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
24	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
23	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
22	Spatial profiling of protein hydrophobicity: native vs. decoy structures. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003 , 52, 561-72	4.2	21
21	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
20	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
19	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, 12777-82	11.5	308
18	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
17	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
16	Blue Gene: A vision for protein science using a petaflop supercomputer. <i>IBM Systems Journal</i> , 2001 , 40, 310-327		175
15	New Linear Interaction Method for Binding Affinity Calculations Using a Continuum Solvent Model. <i>Journal of Physical Chemistry B</i> , 2001 , 105, 10388-10397	3.4	116
14	Poisson-Boltzmann Analytical Gradients for Molecular Modeling Calculations. <i>Journal of Physical Chemistry B</i> , 1999 , 103, 3057-3061	3.4	120
13	Parametrizing a polarizable force field from ab initio data. I. The fluctuating point charge model. <i>Journal of Chemical Physics</i> , 1999 , 110, 741-754	3.9	225
12	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
11	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
10	Smart walking: A new method for Boltzmann sampling of protein conformations. <i>Journal of Chemical Physics</i> , 1997 , 107, 9185-9196	3.9	83
9	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
8	Molecular dynamics for nonequilibrium systems in which there are a small number of very hot particles in a cold bath: Reference system propagator methods. <i>Journal of Chemical Physics</i> , 1996 , 105, 235-239	3.9	2

7	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
6	Adsorption and dissociation of PH ₃ on Si(100)2*1 and Si(111)7*7: Theoretical study. <i>Journal of Physics Condensed Matter</i> , 1994 , 6, 6103-6109	1.8	18
5	Ethylene adsorption and decomposition on Si(100) 2*1: a semi-empirical quantum chemical study. <i>Journal of Physics Condensed Matter</i> , 1993 , 5, 2887-2896	1.8	17
4	The bonding characterization of Br on Si(100)2*1. <i>Journal of Physics Condensed Matter</i> , 1993 , 5, 2897-2902	2.8	5
3	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
2	pi-bonded N ₂ on Cr(110) as a precursor for dissociation: molecular orbital theory. <i>Journal of Physics Condensed Matter</i> , 1992 , 4, 2429-2437	1.8	6
1	Molecular cluster analysis of O ₂ adsorption and dissociation on Pt(111). <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 1992 , 169, 167-172	2.3	9