Qiang Cui

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/581240/publications.pdf

Version: 2024-02-01

		31976	37204
182	10,597	53	96
papers	citations	h-index	g-index

293	293	293	9477
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	DFTB3: Extension of the Self-Consistent-Charge Density-Functional Tight-Binding Method (SCC-DFTB). Journal of Chemical Theory and Computation, 2011, 7, 931-948.	5.3	828
2	Allostery and cooperativity revisited. Protein Science, 2008, 17, 1295-1307.	7.6	603
3	A QM/MM Implementation of the Self-Consistent Charge Density Functional Tight Binding (SCC-DFTB) Method. Journal of Physical Chemistry B, 2001, 105, 569-585.	2.6	568
4	Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications. Chemical Reviews, 2016, 116, 5301-5337.	47.7	312
5	Development of Effective Quantum Mechanical/Molecular Mechanical (QM/MM) Methods for Complex Biological Processes. Journal of Physical Chemistry B, 2006, 110, 6458-6469.	2.6	290
6	Parameterization of DFTB3/3OB for Sulfur and Phosphorus for Chemical and Biological Applications. Journal of Chemical Theory and Computation, 2014, 10, 1518-1537.	5.3	275
7	Extension of the Self-Consistent-Charge Density-Functional Tight-Binding Method:â€‰ Third-Order Expansion of the Density Functional Theory Total Energy and Introduction of a Modified Effective Coulomb Interaction. Journal of Physical Chemistry A, 2007, 111, 10861-10873.	2.5	265
8	Structural insight into substrate preference for TET-mediated oxidation. Nature, 2015, 527, 118-122.	27.8	213
9	A New Coarse-Grained Model for Water: The Importance of Electrostatic Interactions. Journal of Physical Chemistry B, 2010, 114, 10524-10529.	2.6	170
10	A Dynamic Analysis of the Rotation Mechanism for Conformational Change in F1-ATPase. Structure, 2002, 10, 921-931.	3.3	157
11	pKaCalculations in Solution and Proteins with QM/MM Free Energy Perturbation Simulations:Â A Quantitative Test of QM/MM Protocols. Journal of Physical Chemistry B, 2005, 109, 17715-17733.	2.6	157
12	Density functional tight binding: application to organic and biological molecules. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 49-61.	14.6	157
13	Molecular properties from combined QM/MM methods. I. Analytical second derivative and vibrational calculations. Journal of Chemical Physics, 2000, 112, 1133-1149.	3.0	153
14	Modeling zinc in biomolecules with the self consistent charge-density functional tight binding (SCC-DFTB) method: Applications to structural and energetic analysis. Journal of Computational Chemistry, 2003, 24, 565-581.	3.3	150
15	A Normal Mode Analysis of Structural Plasticity in the Biomolecular Motor F1-ATPase. Journal of Molecular Biology, 2004, 340, 345-372.	4.2	149
16	Molecular Properties from Combined QM/MM Methods. 2. Chemical Shifts in Large Molecules. Journal of Physical Chemistry B, 2000, 104, 3721-3743.	2.6	144
17	Specific Reaction Parametrization of the AM1/d Hamiltonian for Phosphoryl Transfer Reactions:â€‰ H, O, and P Atoms. Journal of Chemical Theory and Computation, 2007, 3, 486-504.	5.3	138
18	Parametrization of DFTB3/3OB for Magnesium and Zinc for Chemical and Biological Applications. Journal of Physical Chemistry B, 2015, 119, 1062-1082.	2.6	138

#	Article	IF	Citations
19	â€œProton Holesâ€•in Long-Range Proton Transfer Reactions in Solution and Enzymes:Â A Theoretical Analysis. Journal of the American Chemical Society, 2006, 128, 16302-16311.	13.7	125
20	Density functional tight binding: values of semi-empirical methods in an ab initio era. Physical Chemistry Chemical Physics, 2014, 16, 14368-14377.	2.8	125
21	Quantum Mechanics/Molecular Mechanics Studies of Triosephosphate Isomerase-Catalyzed Reactions:Â Effect of Geometry and Tunneling on Proton-Transfer Rate Constants. Journal of the American Chemical Society, 2002, 124, 3093-3124.	13.7	123
22	Reliable treatment of electrostatics in combined QM/MM simulation of macromolecules. Journal of Chemical Physics, 2005, 123, 014905.	3.0	122
23	Biological Responses to Engineered Nanomaterials: Needs for the Next Decade. ACS Central Science, 2015, 1, 117-123.	11.3	121
24	Structural analysis and modeling reveals new mechanisms governing ESCRT-III spiral filament assembly. Journal of Cell Biology, 2014, 206, 763-777.	5.2	115
25	Importance of van der Waals Interactions in QM/MM Simulations. Journal of Physical Chemistry B, 2004, 108, 6467-6478.	2.6	107
26	Free Energy Perturbation Calculations with Combined QM/MM Potentials Complications, Simplifications, and Applications to Redox Potential Calculations. Journal of Physical Chemistry B, 2003, 107, 8643-8653.	2.6	106
27	Triosephosphate Isomerase:Â A Theoretical Comparison of Alternative Pathways. Journal of the American Chemical Society, 2001, 123, 2284-2290.	13.7	105
28	Dynamics and number of trans-SNARE complexes determine nascent fusion pore properties. Nature, 2018, 554, 260-263.	27.8	103
29	Molecular Simulation of Water and Hydration Effects in Different Environments: Challenges and Developments for DFTB Based Models. Journal of Physical Chemistry B, 2014, 118, 11007-11027.	2.6	97
30	Molecular mechanisms for intrafibrillar collagen mineralization in skeletal tissues. Biomaterials, 2015, 39, 59-66.	11.4	89
31	QM/MM free energy simulations: recent progress and challenges. Molecular Simulation, 2016, 42, 1056-1078.	2.0	89
32	Description of Phosphate Hydrolysis Reactions with the Self-Consistent-Charge Density-Functional-Tight-Binding (SCC-DFTB) Theory. 1. Parameterization. Journal of Chemical Theory and Computation, 2008, 4, 2067-2084.	5.3	87
33	Amino acids with an intermolecular proton bond as proton storage site in bacteriorhodopsin. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 19672-19677.	7.1	87
34	Many Local Motions Cooperate to Produce the Adenylate Kinase Conformational Transition. Journal of Molecular Biology, 2010, 400, 618-631.	4.2	85
35	Application of the SCC-DFTB Method to Neutral and Protonated Water Clusters and Bulk Water. Journal of Physical Chemistry B, 2011, 115, 6790-6805.	2.6	81
36	Proton Transfer in Carbonic Anhydrase Is Controlled by Electrostatics Rather than the Orientation of the Acceptor. Biochemistry, 2008, 47, 2369-2378.	2.5	79

#	Article	IF	Citations
37	Stabilization of Different Types of Transition States in a Single Enzyme Active Site: QM/MM Analysis of Enzymes in the Alkaline Phosphatase Superfamily. Journal of the American Chemical Society, 2013, 135, 10457-10469.	13.7	79
38	Combining implicit solvation models with hybrid quantum mechanical/molecular mechanical methods: A critical test with glycine. Journal of Chemical Physics, 2002, 117, 4720-4728.	3.0	76
39	Perspective: Quantum mechanical methods in biochemistry and biophysics. Journal of Chemical Physics, 2016, 145, 140901.	3.0	76
40	A New Coarse-Grained Force Field for Membraneâ€“Peptide Simulations. Journal of Chemical Theory and Computation, 2011, 7, 3793-3802.	5.3	75
41	Promoting Modes and Demoting Modes in Enzyme-Catalyzed Proton Transfer Reactions:â€‰ A Study of Models and Realistic Systems. Journal of Physical Chemistry B, 2002, 106, 7927-7947.	2.6	74
42	Mechanochemical Coupling in Myosin:Â A Theoretical Analysis with Molecular Dynamics and Combined QM/MM Reaction Path Calculations. Journal of Physical Chemistry B, 2004, 108, 3342-3357.	2.6	74
43	Extensive Conformational Transitions Are Required to Turn On ATP Hydrolysis in Myosin. Journal of Molecular Biology, 2008, 381, 1407-1420.	4.2	71
44	QM/MM Analysis Suggests That Alkaline Phosphatase (AP) and Nucleotide Pyrophosphatase/Phosphodiesterase Slightly Tighten the Transition State for Phosphate Diester Hydrolysis Relative to Solution: Implication for Catalytic Promiscuity in the AP Superfamily. Journal of the American Chemical Society, 2012, 134, 229-246.	13.7	70
45	First-Principles United Atom Force Field for the Ionic Liquid BMIM⁺BF₄^{â€“}: An Alternative to Charge Scaling. Journal of Physical Chemistry B, 2016, 120, 3560-3568.	2.6	68
46	Biomolecular QM/MM Simulations: What Are Some of the â€œBurning Issuesâ€?. Journal of Physical Chemistry B, 2021, 125, 689-702.	2.6	68
47	Catalysis and Specificity in Enzymes: A Study of Triosephosphate Isomerase and Comparison with Methyl Glyoxal Synthase. Advances in Protein Chemistry, 2003, 66, 315-372.	4.4	65
48	Functional plasticity and evolutionary adaptation of allosteric regulation. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 25445-25454.	7.1	65
49	DNMT1 reads heterochromatic H4K20me3 to reinforce LINE-1 DNA methylation. Nature Communications, 2021, 12, 2490.	12.8	63
50	Direct readout of heterochromatic H3K9me3 regulates DNMT1-mediated maintenance DNA methylation. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 18439-18447.	7.1	62
51	Why Do Arginine and Lysine Organize Lipids Differently? Insights from Coarse-Grained and Atomistic Simulations. Journal of Physical Chemistry B, 2013, 117, 12145-12156.	2.6	60
52	Quantum Mechanical/Molecular Mechanical Studies of the Triosephosphate Isomerase-Catalyzed Reaction:â€‰ Verification of Methodology and Analysis of Reaction Mechanisms. Journal of Physical Chemistry B, 2002, 106, 1768-1798.	2.6	58
53	pKaAnalysis for the Zinc-Bound Water in Human Carbonic Anhydrase II:Â Benchmark for â€œMultiscaleâ€• QM/MM Simulations and Mechanistic Implicationsâ€. Journal of Physical Chemistry A, 2007, 111, 5703-5711.	2.5	58
54	Proton Storage Site in Bacteriorhodopsin: New Insights from Quantum Mechanics/Molecular Mechanics Simulations of Microscopic pK_a and Infrared Spectra. Journal of the American Chemical Society, 2011, 133, 14981-14997.	13.7	58

#	Article	IF	Citations
55	Changing hydration level in an internal cavity modulates the proton affinity of a key glutamate in cytochrome c oxidase. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 18886-18891.	7.1	58
56	Microscopic pKa Analysis of Glu286 in Cytochrome c Oxidase (Rhodobacter sphaeroides): Toward a Calibrated Molecular Model. Biochemistry, 2009, 48, 2468-2485.	2.5	57
57	Artificial Intracellular Filaments. Cell Reports Physical Science, 2020, 1, 100085.	5.6	56
58	Different states of synaptotagmin regulate evoked versus spontaneous release. Nature Communications, 2016, 7, 10971.	12.8	53
59	Proton transfer function of carbonic anhydrase: Insights from QM/MM simulations. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2010, 1804, 342-351.	2.3	52
60	Sustainable Nanotechnology: Opportunities and Challenges for Theoretical/Computational Studies. Journal of Physical Chemistry B, 2016, 120, 7297-7306.	2.6	52
61	pK_a of Residue 66 in Staphylococal nuclease. I. Insights from QM/MM Simulations with Conventional Sampling. Journal of Physical Chemistry B, 2008, 112, 8387-8397.	2.6	50
62	Skip residues modulate the structural properties of the myosin rod and guide thick filament assembly. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E3806-15.	7.1	50
63	Improving intermolecular interactions in DFTB3 using extended polarization from chemical-potential equalization. Journal of Chemical Physics, 2015, 143, 084123.	3.0	47
64	Hydrogen-Bond Networks near Supported Lipid Bilayers from Vibrational Sum Frequency Generation Experiments and Atomistic Simulations. Journal of Physical Chemistry B, 2018, 122, 4870-4879.	2.6	47
65	Lipid Corona Formation from Nanoparticle Interactions with Bilayers. CheM, 2018, 4, 2709-2723.	11.7	46
66	Anionic Phospholipids Stabilize RecA Filament Bundles in Escherichia coli. Molecular Cell, 2015, 60, 374-384.	9.7	45
67	N6-methyldeoxyadenosine directs nucleosome positioning in Tetrahymena DNA. Genome Biology, 2018, 19, 200.	8.8	45
68	Mechanochemical Coupling in the Myosin Motor Domain. I. Insights from Equilibrium Active-Site Simulations. PLoS Computational Biology, 2007, 3, e21.	3.2	44
69	The Hydrolysis Activity of Adenosine Triphosphate in Myosin: A Theoretical Analysis of Anomeric Effects and the Nature of the Transition State. Journal of Physical Chemistry A, 2009, 113, 12439-12446.	2.5	43
70	Small moleculeâ€mediated control of hydroxyapatite growth: Free energy calculations benchmarked to density functional theory. Journal of Computational Chemistry, 2014, 35, 70-81.	3.3	42
71	Quantum Effects in Cation Interactions with First and Second Coordination Shell Ligands in Metalloproteins. Journal of Chemical Theory and Computation, 2015, 11, 4992-5001.	5.3	42
72	Structure and dynamics underlying elementary ligand binding events in human pacemaking channels. ELife, 2016, 5, .	6.0	42

#	Article	IF	Citations
73	Microscopic basis for kinetic gating in cytochrome c oxidase: insights from QM/MM analysis. Chemical Science, 2015, 6, 826-841.	7.4	41
74	Infrared spectral marker bands characterizing a transient water wire inside a hydrophobic membrane protein. Journal of Chemical Physics, 2014, 141, 22D524.	3.0	40
75	Predicting the Structureâ€“Activity Relationship of Hydroxyapatite-Binding Peptides by Enhanced-Sampling Molecular Simulation. Langmuir, 2016, 32, 7009-7022.	3.5	39
76	Benchmarking density functional tight binding models for barrier heights and reaction energetics of organic molecules. Journal of Computational Chemistry, 2017, 38, 2171-2185.	3.3	39
77	Leaving Group Ability Observably Affects Transition State Structure in a Single Enzyme Active Site. Journal of the American Chemical Society, 2016, 138, 7386-7394.	13.7	38
78	Quantifying the Electrostatics of Polycationâ€“Lipid Bilayer Interactions. Journal of the American Chemical Society, 2017, 139, 5808-5816.	13.7	38
79	CALCULATING ACCURATE REDOX POTENTIALS IN ENZYMES WITH A COMBINED QM/MM FREE ENERGY PERTURBATION APPROACH. Journal of Theoretical and Computational Chemistry, 2002, 01, 53-67.	1.8	35
80	Regulation and Plasticity of Catalysis in Enzymes: Insights from Analysis of Mechanochemical Coupling in Myosin. Biochemistry, 2017, 56, 1482-1497.	2.5	35
81	Network analysis of a proposed exit pathway for protons to the P-side of cytochrome c oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2018, 1859, 997-1005.	1.0	35
82	An Implicit Solvent Model for SCC-DFTB with Charge-Dependent Radii. Journal of Chemical Theory and Computation, 2010, 6, 2303-2314.	5.3	34
83	Establishing Effective Simulation Protocols for Î²- and Î±/Î²-Mixed Peptides. I. QM and QM/MM Models. Journal of Chemical Theory and Computation, 2007, 3, 1538-1549.	5.3	33
84	Detailed Structure of the H₂PO₄^{â€“}â€“Guanosine Diphosphate Intermediate in Ras-GAP Decoded from FTIR Experiments by Biomolecular Simulations. Journal of the American Chemical Society, 2012, 134, 20041-20044.	13.7	33
85	Substrate and Transition State Binding in Alkaline Phosphatase Analyzed by Computation of Oxygen Isotope Effects. Journal of the American Chemical Society, 2016, 138, 11946-11957.	13.7	33
86	Cavity hydration dynamics in cytochrome c oxidase and functional implications. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E8830-E8836.	7.1	33
87	Large-scale motions in the adenylate kinase solution ensemble: Coarse-grained simulations and comparison with solution X-ray scattering. Chemical Physics, 2012, 396, 84-91.	1.9	32
88	Quantitative Analysis of QM/MM Boundary Artifacts and Correction in Adaptive QM/MM Simulations. Journal of Chemical Theory and Computation, 2019, 15, 3917-3928.	5.3	32
89	A Comparison of Coarse-Grained and Continuum Models for Membrane Bending in Lipid Bilayer Fusion Pores. Biophysical Journal, 2013, 104, 841-852.	0.5	31
90	Microscopic mechanisms that govern the titration response and p K a values of buried residues in staphylococcal nuclease mutants. Proteins: Structure, Function and Bioinformatics, 2017, 85, 268-281.	2.6	31

#	Article	IF	Citations
91	Does Water Relay Play an Important Role in Phosphoryl Transfer Reactions? Insights from Theoretical Study of a Model Reaction in Water and tert-Butanol. Journal of Physical Chemistry B, 2009, 113, 4930-4939.	2.6	30
92	An Explicit Consideration of Desolvation is Critical to Binding Free Energy Calculations of Charged Molecules at Ionic Surfaces. Journal of Chemical Theory and Computation, 2013, 9, 5059-5069.	5.3	30
93	DFTB3 Parametrization for Copper: The Importance of Orbital Angular Momentum Dependence of Hubbard Parameters. Journal of Chemical Theory and Computation, 2015, 11, 4205-4219.	5.3	30
94	The FtsLB subcomplex of the bacterial divisome is a tetramer with an uninterrupted FtsL helix linking the transmembrane and periplasmic regions. Journal of Biological Chemistry, 2018, 293, 1623-1641.	3.4	30
95	A systematic determination of hubbard U using the GBRV ultrasoft pseudopotential set. Computational Materials Science, 2019, 170, 109137.	3.0	30
96	Charging Free Energy Calculations Using the Generalized Solvent Boundary Potential (GSBP) and Periodic Boundary Condition: A Comparative Analysis Using Ion Solvation and Oxidation Free Energy in Proteins. Journal of Physical Chemistry B, 2013, 117, 2005-2018.	2.6	29
97	Proper Thermal Equilibration of Simulations with Drude Polarizable Models: Temperature-Grouped Dual-NosÃ©â€“Hoover Thermostat. Journal of Physical Chemistry Letters, 2019, 10, 7523-7530.	4.6	29
98	Molecular Dynamics Simulation of Interaction between Functionalized Nanoparticles with Lipid Membranes: Analysis of Coarse-Grained Models. Journal of Physical Chemistry B, 2019, 123, 10547-10561.	2.6	26
99	Free Energy Calculations for the Peripheral Binding of Proteins/Peptides to an Anionic Membrane. 1. Implicit Membrane Models. Journal of Chemical Theory and Computation, 2014, 10, 2845-2859.	5.3	25
100	Multiple Pathways and Time Scales for Conformational Transitions in apo-Adenylate Kinase. Journal of Chemical Theory and Computation, 2018, 14, 1716-1726.	5.3	25
101	Three-Dimensional Stress Field around a Membrane Protein: Atomistic andÂCoarse-Grained Simulation Analysis of Gramicidin A. Biophysical Journal, 2013, 104, 117-127.	0.5	24
102	Anionic nanoparticle-induced perturbation to phospholipid membranes affects ion channel function. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 27854-27861.	7.1	24
103	Specific Substates of Ras To Interact with GAPs and Effectors: Revealed by Theoretical Simulations and FTIR Experiments. Journal of Physical Chemistry Letters, 2018, 9, 1312-1317.	4.6	23
104	Counting charges on membrane-bound peptides. Chemical Science, 2018, 9, 4285-4298.	7.4	23
105	Quantum mechanical/molecular mechanical studies of zinc hydrolases. International Reviews in Physical Chemistry, 2014, 33, 1-41.	2.3	22
106	Towards a barrier height benchmark set for biologically relevant systems. PeerJ, 2016, 4, e1994.	2.0	22
107	Copper Oxidation/Reduction in Water and Protein: Studies with DFTB3/MM and VALBOND Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2016, 120, 1894-1910.	2.6	22
108	A computational investigation on the substrate preference of ten-eleven-translocation 2 (TET2). Physical Chemistry Chemical Physics, 2016, 18, 4728-4738.	2.8	21

#	Article	IF	Citations
109	Cholesterol Interaction with the Trimeric HIV Fusion Protein gp41 in Lipid Bilayers Investigated by Solid-State NMR Spectroscopy and Molecular Dynamics Simulations. Journal of Molecular Biology, 2020, 432, 4705-4721.	4.2	21
110	Ionic Hydrogen Bonds and Lipid Packing Defects Determine the Binding Orientation and Insertion Depth of RecA on Multicomponent Lipid Bilayers. Journal of Physical Chemistry B, 2016, 120, 8424-8437.	2.6	20
111	Extensive free-energy simulations identify water as the base in nucleotide addition by DNA polymerase. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 25048-25056.	7.1	20
112	Interconversion of Functional Motions between Mesophilic and Thermophilic Adenylate Kinases. PLoS Computational Biology, 2011, 7, e1002103.	3.2	19
113	Generation and sensing of membrane curvature: Where materials science and biophysics meet. Current Opinion in Solid State and Materials Science, 2013, 17, 164-174.	11.5	19
114	Comparison of native and non-native ubiquitin oligomers reveals analogous structures and reactivities. Protein Science, 2016, 25, 456-471.	7.6	18
115	Essence of Small Molecule-Mediated Control of Hydroxyapatite Growth: Free Energy Calculations of Amino Acid Side Chain Analogues. Journal of Physical Chemistry C, 2018, 122, 4372-4380.	3.1	17
116	Specificity landscapes unmask submaximal binding site preferences of transcription factors. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E10586-E10595.	7.1	16
117	Structural and mechanistic basis for preferential deadenylation of U6 snRNA by Usb1. Nucleic Acids Research, 2018, 46, 11488-11501.	14.5	16
118	Conformational and Dynamic Properties of Poly(ethylene oxide) in BMIM⁺BF₄^{â€“}: A Microsecond Computer Simulation Study Using ab Initio Force Fields. Macromolecules, 2018, 51, 5336-5345.	4.8	16
119	Protein-induced membrane curvature in coarse-grained simulations. Biophysical Journal, 2021, 120, 3211-3221.	0.5	16
120	Coacervation of poly-electrolytes in the presence of lipid bilayers: mutual alteration of structure and morphology. Chemical Science, 2022, 13, 7933-7946.	7.4	16
121	Molecular Dynamics Simulations Establish the Molecular Basis for the Broad Allostery Hotspot Distributions in the Tetracycline Repressor. Journal of the American Chemical Society, 2022, 144, 10870-10887.	13.7	16
122	The histone H3 N-terminal tail: a computational analysis of the free energy landscape and kinetics. Physical Chemistry Chemical Physics, 2015, 17, 13689-13698.	2.8	15
123	A composite approach towards a complete model of the myosin rod. Proteins: Structure, Function and Bioinformatics, 2016, 84, 172-189.	2.6	15
124	Analysis of the conformational properties of amine ligands at the gold/water interface with QM, MM and QM/MM simulations. Physical Chemistry Chemical Physics, 2018, 20, 3349-3362.	2.8	15
125	Electrostatics, Hydrogen Bonding, and Molecular Structure at Polycation and Peptide:Lipid Membrane Interfaces. ACS Applied Materials & Interfaces, 2020, 12, 21149-21158.	8.0	15
126	Single-Step Replacement of an Unreactive Câ€“H Bond by a Câ€“S Bond Using Polysulfide as the Direct Sulfur Source in the Anaerobic Ergothioneine Biosynthesis. ACS Catalysis, 2020, 10, 8981-8994.	11.2	15

#	Article	IF	Citations
127	Substrate deformation regulates DRM2-mediated DNA methylation in plants. Science Advances, 2021, 7, .	10.3	15
128	The complexin C-terminal amphipathic helix stabilizes the fusion pore open state by sculpting membranes. Nature Structural and Molecular Biology, 2022, 29, 97-107.	8.2	15
129	A Hybrid Molecular Dynamics/Multiconformer Continuum Electrostatics (MD/MCCE) Approach for the Determination of Surface Charge of Nanomaterials. Journal of Physical Chemistry C, 2017, 121, 3584-3596.	3.1	14
130	Interfacial water and ion distribution determine Î¶ potential and binding affinity of nanoparticles to biomolecules. Nanoscale, 2020, 12, 18106-18123.	5.6	14
131	Molecular Simulation of Mechanical Properties and Membrane Activities of the ESCRT-III Complexes. Biophysical Journal, 2020, 118, 1333-1343.	0.5	14
132	Exploring the applicability of density functional tight binding to transition metal ions. Parameterization for nickel with the spinâ€polarized DFTB3 model. Journal of Computational Chemistry, 2019, 40, 400-413.	3.3	13
133	Multi-level free energy simulation with a staged transformation approach. Journal of Chemical Physics, 2020, 153, 044115.	3.0	13
134	Identifying the proton loading site cluster in the ba cytochrome c oxidase that loads and traps protons. Biochimica Et Biophysica Acta - Bioenergetics, 2020, 1861, 148239.	1.0	13
135	Allosteric Activation Transitions in Enzymes and Biomolecular Motors: Insights from Atomistic and Coarse-Grained Simulations. Topics in Current Chemistry, 2013, 337, 139-164.	4.0	12
136	Implications for an Imidazole-2-yl Carbene Intermediate in the Rhodanase-Catalyzed Câ€“S Bond Formation Reaction of Anaerobic Ergothioneine Biosynthesis. ACS Catalysis, 2021, 11, 3319-3334.	11.2	12
137	Conformational Features of Ras: Key Hydrogen-Bonding Interactions of Gln61 in the Intermediate State during GTP Hydrolysis. Journal of Physical Chemistry B, 2021, 125, 8805-8813.	2.6	12
138	Unconventional aliphatic fluorophores discovered as the luminescence origin in citric acidâ€“urea carbon dots. Nanoscale, 2022, 14, 9516-9525.	5.6	12
139	Self-Assembly of Î²-Peptides: Insight from the Pair and Many-Body Free Energy of Association. Journal of Physical Chemistry C, 2010, 114, 13551-13556.	3.1	11
140	Tethered Spectroscopic Probes Estimate Dynamic Distances with Subnanometer Resolution in Voltage-Dependent Potassium Channels. Biophysical Journal, 2013, 105, 2724-2732.	0.5	11
141	Analysis of Phosphoryl-Transfer Enzymes with QM/MM Free Energy Simulations. Methods in Enzymology, 2018, 607, 53-90.	1.0	11
142	Multiple deprotonation paths of the nucleophile 3â€²-OH in the DNA synthesis reaction. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, e2103990118.	7.1	11
143	Gating mechanism of mechanosensitive channel of large conductance: a coupled continuum mechanical-continuum solvation approach. Biomechanics and Modeling in Mechanobiology, 2016, 15, 1557-1576.	2.8	10
144	Small Molecule Chelators Reveal That Iron Starvation Inhibits Late Stages of Bacterial Cytokinesis. ACS Chemical Biology, 2018, 13, 235-246.	3.4	10

#	Article	IF	Citations
145	Intermolecular interactions in the condensed phase: Evaluation of semi-empirical quantum mechanical methods. Journal of Chemical Physics, 2017, 147, 161704.	3.0	9
146	Interfacial Polarization and Ionic Structure at the Ionic Liquidâ€“Metal Interface Studied by Vibrational Spectroscopy and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2021, 125, 2741-2753.	2.6	9
147	Identification of functional substates of KRas during GTP hydrolysis with enhanced sampling simulations. Physical Chemistry Chemical Physics, 2022, 24, 7653-7665.	2.8	9
148	Factors That Determine the Variation of Equilibrium and Kinetic Properties of QM/MM Enzyme Simulations: QM Region, Conformation, and Boundary Condition. Journal of Chemical Theory and Computation, 2022, 18, 2530-2542.	5.3	9
149	Conformations and binding pockets of <scp>HRas</scp> and its guanine nucleotide exchange factors complexes in the guanosine triphosphate exchange process. Journal of Computational Chemistry, 2022, 43, 906-916.	3.3	9
150	Toward molecular models of proton pumping: Challenges, methods and relevant applications. Science China Chemistry, 2012, 55, 3-18.	8.2	8
151	Ligand Length and Surface Curvature Modulate Nanoparticle Surface Heterogeneity and Electrostatics. Journal of Physical Chemistry C, 2020, 124, 24513-24525.	3.1	8
152	The coiled-coil domain of Escherichia coli FtsLB is a structurally detuned element critical for modulating its activation in bacterial cell division. Journal of Biological Chemistry, 2022, 298, 101460.	3.4	8
153	Mapping temperature-dependent conformational change in the voltage-sensing domain of an engineered heat-activated K ⁺ channel. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	7
154	Electronic Polarization Is Essential for the Stabilization and Dynamics of Buried Ion Pairs in Staphylococcal Nuclease Mutants. Journal of the American Chemical Society, 2022, 144, 4594-4610.	13.7	7
155	Multiple gas-phase conformations of proline-containing peptides: is it always cis/trans isomerization?. Analyst, The, 2016, 141, 4863-4869.	3.5	6
156	Analysis of Density Functional Tight Binding with Natural Bonding Orbitals. Journal of Physical Chemistry A, 2019, 123, 7439-7453.	2.5	6
157	Influence of Surface Ligand Molecular Structure on Phospholipid Membrane Disruption by Cationic Nanoparticles. Langmuir, 2021, 37, 7600-7610.	3.5	6
158	â€œMulti-Scaleâ€•QM/MM Methods with Self-Consistent-Charge Density-Functional-Tight-Binding (SCC-DFTB). Challenges and Advances in Computational Chemistry and Physics, 2009, , 173-196.	0.6	6
159	Title is missing!. Angewandte Chemie, 2003, 115, 1546-1549.	2.0	5
160	Making Biomolecular Simulations Accessible in the Post-Nobel Prize Era. PLoS Computational Biology, 2014, 10, e1003786.	3.2	5
161	Protonation-Driven Aqueous Lyotropic Self-Assembly of Synthetic Six-Tail Lipidoids. Langmuir, 2020, 36, 8240-8252.	3.5	5
162	O to bR transition in bacteriorhodopsin occurs through a proton hole mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	5

#	Article	IF	Citations
163	Differences in the Nature of the Phosphoryl Transfer Transition State in Protein Phosphatase 1 and Alkaline Phosphatase: Insights from QM Cluster Models. Journal of Physical Chemistry B, 2020, 124, 9371-9384.	2.6	4
164	Modulation of Nanoparticle Diffusion by Surface Ligand Length and Charge: Analysis with Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2021, 125, 4555-4565.	2.6	4
165	Reverse Protonation of Buried Ion-Pairs in Staphylococcal Nuclease Mutants. Journal of Chemical Theory and Computation, 2021, 17, 4550-4563.	5.3	4
166	Cholesterol-Mediated Clustering of the HIV Fusion Protein gp41 in Lipid Bilayers. Journal of Molecular Biology, 2022, 434, 167345.	4.2	4
167	Machine Learning-Assisted Phase Transition Temperatures from Generalized Replica Exchange Simulations of Dry Martini Lipid Bilayers. Journal of Physical Chemistry Letters, 2022, 13, 6481-6486.	4.6	4
168	Membrane-mediated interaction drives mitochondrial ATPase assembly and cristae formation. Journal of General Physiology, 2018, 150, 777-780.	1.9	3
169	NMR Structural Analysis of Isolated Shaker Voltage-Sensing Domain in LPPG Micelles. Biophysical Journal, 2019, 117, 388-398.	0.5	3
170	What Does the BrÃ¸nsted Slope Measure in the Phosphoryl Transfer Transition State?. ACS Catalysis, 2020, 10, 13932-13945.	11.2	3
171	Improvement of dâ€“d interactions in density functional tight binding for transition metal ions with a ligand field model: assessment of a DFTB3+U model on nickel coordination compounds. Physical Chemistry Chemical Physics, 2020, 22, 27084-27095.	2.8	3
172	Interplay of Electrostatics and Hydrophobic Effects in the Metamorphic Protein Human Lymphotactin. Journal of Physical Chemistry B, 2015, 119, 9547-9558.	2.6	2
173	Gating and inactivation of mechanosensitive channels of small conductance: A continuum mechanics study. Journal of the Mechanical Behavior of Biomedical Materials, 2019, 90, 502-514.	3.1	2
174	Binding of polar and hydrophobic molecules at the LiCoO₂ (001)-water interface: force field development and molecular dynamics simulations. Nanoscale, 2022, , .	5.6	2
175	Electronic Structure of de Novo Peptide ACC-Hex from First Principles. Journal of Physical Chemistry B, 2022, 126, 4289-4298.	2.6	2
176	Cover Image, Volume 85, Issue 2. Proteins: Structure, Function and Bioinformatics, 2017, 85, C4-C4.	2.6	0
177	Antibiotic Resistance: Photoâ€Disassembly of Membrane Microdomains Revives Conventional Antibiotics against MRSA (Adv. Sci. 6/2020). Advanced Science, 2020, 7, 2070035.	11.2	0
178	Viewpoint on ACS PHYS Division Sponsored Virtual Seminars. Journal of Physical Chemistry C, 2021, 125, 4342-4342.	3.1	0
179	Viewpoint on ACS PHYS Division Sponsored Virtual Seminars. Journal of Physical Chemistry A, 2021, 125, 1680-1680.	2.5	0
180	Viewpoint on ACS PHYS Division Sponsored Virtual Seminars. Journal of Physical Chemistry B, 2021, 125, 1973-1973.	2.6	0

#	Article	IF	Citations
181	Structural organization of the FtsLB complex of the bacterial divisome. FASEB Journal, 2019, 33, .	0.5	0
182	Editorial overview: Theory and simulation: Molecular modeling from atoms to complexes. Current Opinion in Structural Biology, 2022, 73, 102347.	5.7	0