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	Cholesterol-Mediated Clustering of the HIV Fusion Protein gp41 in Lipid Bilayers. Journal of Molecular Biology, 2022, 434, 167345.	4.2	4
2	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
3	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
4	Identification of functional substates of KRas during GTP hydrolysis with enhanced sampling simulations. Physical Chemistry Chemical Physics, 2022, 24, 7653-7665.	2.8	9
5	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
6	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
7	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
8	Editorial overview: Theory and simulation: Molecular modeling from atoms to complexes. Current Opinion in Structural Biology, 2022, 73, 102347.	5.7	0
9	Binding of polar and hydrophobic molecules at the LiCoO₂ (001)-water interface: force field development and molecular dynamics simulations. Nanoscale, 2022, , .	5.6	2
10	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
11	Unconventional aliphatic fluorophores discovered as the luminescence origin in citric acidâ€“urea carbon dots. Nanoscale, 2022, 14, 9516-9525.	5.6	12
12	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
13	Electronic Structure of de Novo Peptide ACC-Hex from First Principles. Journal of Physical Chemistry B, 2022, 126, 4289-4298.	2.6	2
14	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
15	Biomolecular QM/MM Simulations: What Are Some of the â€œBurning Issuesâ€?. Journal of Physical Chemistry B, 2021, 125, 689-702.	2.6	68
16	Viewpoint on ACS PHYS Division Sponsored Virtual Seminars. Journal of Physical Chemistry C, 2021, 125, 4342-4342.	3.1	0
17	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
18	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

#	Article	IF	Citations
19	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
20	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
21	DNMT1 reads heterochromatic H4K20me3 to reinforce LINE-1 DNA methylation. Nature Communications, 2021, 12, 2490.	12.8	63
22	Reverse Protonation of Buried Ion-Pairs in Staphylococcal Nuclease Mutants. Journal of Chemical Theory and Computation, 2021, 17, 4550-4563.	5.3	4
23	Influence of Surface Ligand Molecular Structure on Phospholipid Membrane Disruption by Cationic Nanoparticles. Langmuir, 2021, 37, 7600-7610.	3.5	6
24	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
25	Substrate deformation regulates DRM2-mediated DNA methylation in plants. Science Advances, 2021, 7, .	10.3	15
26	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
27	Protein-induced membrane curvature in coarse-grained simulations. Biophysical Journal, 2021, 120, 3211-3221.	0.5	16
28	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
29	Viewpoint on ACS PHYS Division Sponsored Virtual Seminars. Journal of Physical Chemistry A, 2021, 125, 1680-1680.	2.5	0
30	Viewpoint on ACS PHYS Division Sponsored Virtual Seminars. Journal of Physical Chemistry B, 2021, 125, 1973-1973.	2.6	0
31	Electrostatics, Hydrogen Bonding, and Molecular Structure at Polycation and Peptide:Lipid Membrane Interfaces. ACS Applied Materials & Interfaces, 2020, 12, 21149-21158.	8.0	15
32	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
33	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
34	What Does the BrÃ¸nsted Slope Measure in the Phosphoryl Transfer Transition State?. ACS Catalysis, 2020, 10, 13932-13945.	11.2	3
35	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
36	Ligand Length and Surface Curvature Modulate Nanoparticle Surface Heterogeneity and Electrostatics. Journal of Physical Chemistry C, 2020, 124, 24513-24525.	3.1	8

#	Article	IF	Citations
37	Interfacial water and ion distribution determine Î¶ potential and binding affinity of nanoparticles to biomolecules. Nanoscale, 2020, 12, 18106-18123.	5.6	14
38	Multi-level free energy simulation with a staged transformation approach. Journal of Chemical Physics, 2020, 153, 044115.	3.0	13
39	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
40	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
41	Antibiotic Resistance: Photoâ€Disassembly of Membrane Microdomains Revives Conventional Antibiotics against MRSA (Adv. Sci. 6/2020). Advanced Science, 2020, 7, 2070035.	11.2	0
42	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
43	Artificial Intracellular Filaments. Cell Reports Physical Science, 2020, 1, 100085.	5.6	56
44	Protonation-Driven Aqueous Lyotropic Self-Assembly of Synthetic Six-Tail Lipidoids. Langmuir, 2020, 36, 8240-8252.	3.5	5
45	Molecular Simulation of Mechanical Properties and Membrane Activities of the ESCRT-III Complexes. Biophysical Journal, 2020, 118, 1333-1343.	0.5	14
46	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
47	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
48	Analysis of Density Functional Tight Binding with Natural Bonding Orbitals. Journal of Physical Chemistry A, 2019, 123, 7439-7453.	2.5	6
49	A systematic determination of hubbard U using the GBRV ultrasoft pseudopotential set. Computational Materials Science, 2019, 170, 109137.	3.0	30
50	NMR Structural Analysis of Isolated Shaker Voltage-Sensing Domain in LPPG Micelles. Biophysical Journal, 2019, 117, 388-398.	0.5	3
51	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
52	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
53	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
54	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

#	Article	IF	Citations
55	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
56	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
57	Structural organization of the FtsLB complex of the bacterial divisome. FASEB Journal, 2019, 33, .	0.5	0
58	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
59	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
60	Counting charges on membrane-bound peptides. Chemical Science, 2018, 9, 4285-4298.	7.4	23
61	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
62	Dynamics and number of trans-SNARE complexes determine nascent fusion pore properties. Nature, 2018, 554, 260-263.	27.8	103
63	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
64	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
65	Small Molecule Chelators Reveal That Iron Starvation Inhibits Late Stages of Bacterial Cytokinesis. ACS Chemical Biology, 2018, 13, 235-246.	3.4	10
66	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
67	Membrane-mediated interaction drives mitochondrial ATPase assembly and cristae formation. Journal of General Physiology, 2018, 150, 777-780.	1.9	3
68	N6-methyldeoxyadenosine directs nucleosome positioning in Tetrahymena DNA. Genome Biology, 2018, 19, 200.	8.8	45
69	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
70	Lipid Corona Formation from Nanoparticle Interactions with Bilayers. CheM, 2018, 4, 2709-2723.	11.7	46
71	Structural and mechanistic basis for preferential deadenylation of U6 snRNA by Usb1. Nucleic Acids Research, 2018, 46, 11488-11501.	14.5	16
72	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

#	Article	IF	Citations
73	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
74	Analysis of Phosphoryl-Transfer Enzymes with QM/MM Free Energy Simulations. Methods in Enzymology, 2018, 607, 53-90.	1.0	11
75	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
76	Regulation and Plasticity of Catalysis in Enzymes: Insights from Analysis of Mechanochemical Coupling in Myosin. Biochemistry, 2017, 56, 1482-1497.	2.5	35
77	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
78	Intermolecular interactions in the condensed phase: Evaluation of semi-empirical quantum mechanical methods. Journal of Chemical Physics, 2017, 147, 161704.	3.0	9
79	Quantifying the Electrostatics of Polycationâ€“Lipid Bilayer Interactions. Journal of the American Chemical Society, 2017, 139, 5808-5816.	13.7	38
80	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
81	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
82	Cover Image, Volume 85, Issue 2. Proteins: Structure, Function and Bioinformatics, 2017, 85, C4-C4.	2.6	0
83	Towards a barrier height benchmark set for biologically relevant systems. PeerJ, 2016, 4, e1994.	2.0	22
84	Comparison of native and non-native ubiquitin oligomers reveals analogous structures and reactivities. Protein Science, 2016, 25, 456-471.	7.6	18
85	Predicting the Structureâ€“Activity Relationship of Hydroxyapatite-Binding Peptides by Enhanced-Sampling Molecular Simulation. Langmuir, 2016, 32, 7009-7022.	3.5	39
86	QM/MM free energy simulations: recent progress and challenges. Molecular Simulation, 2016, 42, 1056-1078.	2.0	89
87	Perspective: Quantum mechanical methods in biochemistry and biophysics. Journal of Chemical Physics, 2016, 145, 140901.	3.0	76
88	A composite approach towards a complete model of the myosin rod. Proteins: Structure, Function and Bioinformatics, 2016, 84, 172-189.	2.6	15
89	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
90	Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications. Chemical Reviews, 2016, 116, 5301-5337.	47.7	312

#	Article	IF	Citations
91	Multiple gas-phase conformations of proline-containing peptides: is it always cis/trans isomerization?. Analyst, The, 2016, 141, 4863-4869.	3.5	6
92	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
93	Sustainable Nanotechnology: Opportunities and Challenges for Theoretical/Computational Studies. Journal of Physical Chemistry B, 2016, 120, 7297-7306.	2.6	52
94	Different states of synaptotagmin regulate evoked versus spontaneous release. Nature Communications, 2016, 7, 10971.	12.8	53
95	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
96	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
97	A computational investigation on the substrate preference of ten-eleven-translocation 2 (TET2). Physical Chemistry Chemical Physics, 2016, 18, 4728-4738.	2.8	21
98	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
99	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
100	Structure and dynamics underlying elementary ligand binding events in human pacemaking channels. ELife, 2016, 5, .	6.0	42
101	Improving intermolecular interactions in DFTB3 using extended polarization from chemical-potential equalization. Journal of Chemical Physics, 2015, 143, 084123.	3.0	47
102	Biological Responses to Engineered Nanomaterials: Needs for the Next Decade. ACS Central Science, 2015, 1, 117-123.	11.3	121
103	Interplay of Electrostatics and Hydrophobic Effects in the Metamorphic Protein Human Lymphotactin. Journal of Physical Chemistry B, 2015, 119, 9547-9558.	2.6	2
104	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
105	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
106	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
107	Structural insight into substrate preference for TET-mediated oxidation. Nature, 2015, 527, 118-122.	27.8	213
108	Anionic Phospholipids Stabilize RecA Filament Bundles in Escherichia coli. Molecular Cell, 2015, 60, 374-384.	9.7	45

#	Article	IF	Citations
109	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
110	Molecular mechanisms for intrafibrillar collagen mineralization in skeletal tissues. Biomaterials, 2015, 39, 59-66.	11.4	89
111	Microscopic basis for kinetic gating in cytochrome c oxidase: insights from QM/MM analysis. Chemical Science, 2015, 6, 826-841.	7.4	41
112	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
113	Making Biomolecular Simulations Accessible in the Post-Nobel Prize Era. PLoS Computational Biology, 2014, 10, e1003786.	3.2	5
114	Infrared spectral marker bands characterizing a transient water wire inside a hydrophobic membrane protein. Journal of Chemical Physics, 2014, 141, 22D524.	3.0	40
115	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
116	Quantum mechanical/molecular mechanical studies of zinc hydrolases. International Reviews in Physical Chemistry, 2014, 33, 1-41.	2.3	22
117	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
118	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
119	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
120	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
121	Structural analysis and modeling reveals new mechanisms governing ESCRT-III spiral filament assembly. Journal of Cell Biology, 2014, 206, 763-777.	5.2	115
122	Density functional tight binding: application to organic and biological molecules. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 49-61.	14.6	157
123	Tethered Spectroscopic Probes Estimate Dynamic Distances with Subnanometer Resolution in Voltage-Dependent Potassium Channels. Biophysical Journal, 2013, 105, 2724-2732.	0.5	11
124	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
125	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
126	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

#	Article	IF	Citations
127	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
128	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
129	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
130	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
131	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
132	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
133	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
134	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
135	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
136	Toward molecular models of proton pumping: Challenges, methods and relevant applications. Science China Chemistry, 2012, 55, 3-18.	8.2	8
137	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
138	A New Coarse-Grained Force Field for Membraneâ€“Peptide Simulations. Journal of Chemical Theory and Computation, 2011, 7, 3793-3802.	5.3	75
139	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
140	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
141	Interconversion of Functional Motions between Mesophilic and Thermophilic Adenylate Kinases. PLoS Computational Biology, 2011, 7, e1002103.	3.2	19
142	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
143	A New Coarse-Grained Model for Water: The Importance of Electrostatic Interactions. Journal of Physical Chemistry B, 2010, 114, 10524-10529.	2.6	170
144	An Implicit Solvent Model for SCC-DFTB with Charge-Dependent Radii. Journal of Chemical Theory and Computation, 2010, 6, 2303-2314.	5.3	34

#	Article	IF	Citations
145	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
146	Many Local Motions Cooperate to Produce the Adenylate Kinase Conformational Transition. Journal of Molecular Biology, 2010, 400, 618-631.	4.2	85
147	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
148	Microscopic pKa Analysis of Glu286 in Cytochrome c Oxidase (Rhodobacter sphaeroides): Toward a Calibrated Molecular Model. Biochemistry, 2009, 48, 2468-2485.	2.5	57
149	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
150	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
151	Allostery and cooperativity revisited. Protein Science, 2008, 17, 1295-1307.	7.6	603
152	Extensive Conformational Transitions Are Required to Turn On ATP Hydrolysis in Myosin. Journal of Molecular Biology, 2008, 381, 1407-1420.	4.2	71
153	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
154	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
155	Proton Transfer in Carbonic Anhydrase Is Controlled by Electrostatics Rather than the Orientation of the Acceptor. Biochemistry, 2008, 47, 2369-2378.	2.5	79
156	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
157	Mechanochemical Coupling in the Myosin Motor Domain. I. Insights from Equilibrium Active-Site Simulations. PLoS Computational Biology, 2007, 3, e21.	3.2	44
158	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
159	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
160	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
161	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
162	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

#	Article	IF	Citations
163	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
164	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
165	Reliable treatment of electrostatics in combined QM/MM simulation of macromolecules. Journal of Chemical Physics, 2005, 123, 014905.	3.0	122
166	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
167	Importance of van der Waals Interactions in QM/MM Simulations. Journal of Physical Chemistry B, 2004, 108, 6467-6478.	2.6	107
168	A Normal Mode Analysis of Structural Plasticity in the Biomolecular Motor F1-ATPase. Journal of Molecular Biology, 2004, 340, 345-372.	4.2	149
169	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
170	Title is missing!. Angewandte Chemie, 2003, 115, 1546-1549.	2.0	5
171	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
172	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
173	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
174	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
175	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
176	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
177	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
178	A Dynamic Analysis of the Rotation Mechanism for Conformational Change in F1-ATPase. Structure, 2002, 10, 921-931.	3.3	157
179	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
180	Triosephosphate Isomerase:Â A Theoretical Comparison of Alternative Pathways. Journal of the American Chemical Society, 2001, 123, 2284-2290.	13.7	105

#	Article	IF	Citations
181	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
182	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