Qiang Cui

List of Publications by Year in Descending Order

166 papers	8,534 citations	51 h-index	88 g-index
293 ext. papers	9,738 ext. citations	7.3 avg, IF	6.5 L-index

#	Paper	IF	Citations
166	Cholesterol-Mediated Clustering of the HIV Fusion Protein gp41 in Lipid Bilayers. *Journal of Molecular Biology*, **2021**, 434, 167345	6.5	1
165	Computational Studies of Enzyme Motions **2021**, 1-9		
164	The coiled-coil domain of E. coli FtsLB is a structurally detuned element critical for modulating its activation in bacterial cell division. *Journal of Biological Chemistry*, **2021**, 101460	5.4	0
163	Interfacial Polarization and Ionic Structure at the Ionic Liquid-Metal Interface Studied by Vibrational Spectroscopy and Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2021**, 125, 2741-2753	3.4	5
162	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,	11.5	3
161	Implications for an imidazol-2-yl carbene intermediate in the rhodanase-catalyzed C-S bond formation reaction of anaerobic ergothioneine biosynthesis. *ACS Catalysis*, **2021**, 11, 3319-3334	13.1	2
160	Modulation of Nanoparticle Diffusion by Surface Ligand Length and Charge: Analysis with Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2021**, 125, 4555-4565	3.4	1
159	DNMT1 reads heterochromatic H4K20me3 to reinforce LINE-1 DNA methylation. *Nature Communications*, **2021**, 12, 2490	17.4	13
158	Reverse Protonation of Buried Ion-Pairs in Staphylococcal Nuclease Mutants. *Journal of Chemical Theory and Computation*, **2021**, 17, 4550-4563	6.4	1
157	Influence of Surface Ligand Molecular Structure on Phospholipid Membrane Disruption by Cationic Nanoparticles. *Langmuir*, **2021**, 37, 7600-7610	4	2
156	Multiple deprotonation paths of the nucleophile 3'-OH in the DNA synthesis reaction. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	2
155	Substrate deformation regulates DRM2-mediated DNA methylation in plants. *Science Advances*, **2021**, 7,	14.3	2
154	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	3.4	6
153	Biomolecular QM/MM Simulations: What Are Some of the "Burning Issues"?. *Journal of Physical Chemistry B*, **2021**, 125, 689-702	3.4	22
152	Viewpoint on ACS PHYS Division Sponsored Virtual Seminars. *Journal of Physical Chemistry C*, **2021**, 125, 4342-4342	3.8	
151	Protein-induced membrane curvature in coarse-grained simulations. *Biophysical Journal*, **2021**, 120, 3211-3221	3.4	1
150	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	3.4	3

149	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	6.5	12
148	Antibiotic Resistance: Photo-Disassembly of Membrane Microdomains Revives Conventional Antibiotics against MRSA (Adv. Sci. 6/2020). *Advanced Science*, **2020**, 7, 2070035	13.6	78
147	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	4.6	6
146	Artificial Intracellular Filaments. *Cell Reports Physical Science*, **2020**, 1,	6.1	37
145	Protonation-Driven Aqueous Lyotropic Self-Assembly of Synthetic Six-Tail Lipidoids. *Langmuir*, **2020** , 36, 8240-8252	4	1
144	Molecular Simulation of Mechanical Properties and Membrane Activities of the ESCRT-III Complexes. *Biophysical Journal*, **2020**, 118, 1333-1343	2.9	5
143	Improvement of d-d interactions in density functional tight binding for transition metal ions with a ligand field model: assessment of a DFTB3+ model on nickel coordination compounds. *Physical Chemistry Chemical Physics*, **2020**, 22, 27084-27095	3.6	2
142	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	11.5	30
141	Electrostatics, Hydrogen Bonding, and Molecular Structure at Polycation and Peptide:Lipid Membrane Interfaces. *ACS Applied Materials & Interfaces*, **2020**, 12, 21149-21158	9.5	8
140	Single-step Replacement of an Unreactive C-H Bond by a C-S Bond Using Polysulfide as the Direct Sulfur Source in Anaerobic Ergothioneine Biosynthesis. *ACS Catalysis*, **2020**, 10, 8981-8994	13.1	6
139	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	11.5	26
138	What Does the Brønsted Slope Measure in the Phosphoryl Transfer Transition State?. *ACS Catalysis*, **2020**, 10, 13932-13945	13.1	2
137	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	11.5	8
136	Ligand Length and Surface Curvature Modulate Nanoparticle Surface Heterogeneity and Electrostatics. *Journal of Physical Chemistry C*, **2020**, 124, 24513-24525	3.8	1
135	Interfacial water and ion distribution determine potential and binding affinity of nanoparticles to biomolecules. *Nanoscale*, **2020**, 12, 18106-18123	7.7	6
134	Multi-level free energy simulation with a staged transformation approach. *Journal of Chemical Physics*, **2020**, 153, 044115	3.9	6
133	Quantitative Analysis of QM/MM Boundary Artifacts and Correction in Adaptive QM/MM Simulations. *Journal of Chemical Theory and Computation*, **2019**, 15, 3917-3928	6.4	21
132	Analysis of Density Functional Tight Binding with Natural Bonding Orbitals. *Journal of Physical Chemistry A*, **2019**, 123, 7439-7453	2.8	4

131	A systematic determination of hubbard U using the GBRV ultrasoft pseudopotential set. *Computational Materials Science*, **2019**, 170, 109137	3.2	11
130	NMR Structural Analysis of Isolated Shaker Voltage-Sensing Domain in LPPG Micelles. *Biophysical Journal*, **2019**, 117, 388-398	2.9	3
129	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	3.4	15
128	Proper Thermal Equilibration of Simulations with Drude Polarizable Models: Temperature-Grouped Dual-Nos□Hoover Thermostat. *Journal of Physical Chemistry Letters*, **2019**, 10, 7523-7530	6.4	12
127	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	11.5	9
126	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	4.1	2
125	Exploring the applicability of density functional tight binding to transition metal ions. Parameterization for nickel with the spin-polarized DFTB3 model. *Journal of Computational Chemistry*, **2019**, 40, 400-413	3.5	11
124	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	6.4	14
123	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	3.4	40
122	Counting charges on membrane-bound peptides. *Chemical Science*, **2018**, 9, 4285-4298	9.4	21
121	Multiple Pathways and Time Scales for Conformational Transitions in apo-Adenylate Kinase. *Journal of Chemical Theory and Computation*, **2018**, 14, 1716-1726	6.4	13
120	Dynamics and number of trans-SNARE complexes determine nascent fusion pore properties. *Nature* , **2018**, 554, 260-263	50.4	56
119	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	3.8	14
118	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	5.4	11
117	Conformational and Dynamic Properties of Poly(ethylene oxide) in BMIM+BF4□A Microsecond Computer Simulation Study Using ab Initio Force Fields. *Macromolecules*, **2018**, 51, 5336-5345	5.5	12
116	Analysis of Phosphoryl-Transfer Enzymes with QM/MM Free Energy Simulations. *Methods in Enzymology*, **2018**, 607, 53-90	1.7	8
115	Small Molecule Chelators Reveal That Iron Starvation Inhibits Late Stages of Bacterial Cytokinesis. *ACS Chemical Biology*, **2018**, 13, 235-246	4.9	8
114	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	3.6	12

113	Membrane-mediated interaction drives mitochondrial ATPase assembly and cristae formation. *Journal of General Physiology*, **2018**, 150, 777-780	3.4	3
112	N-methyldeoxyadenosine directs nucleosome positioning in Tetrahymena DNA. *Genome Biology*, **2018**, 19, 200	18.3	26
111	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	11.5	7
110	Lipid Corona Formation from Nanoparticle Interactions with Bilayers. *CheM*, **2018**, 4, 2709-2723	16.2	28
109	Structural and mechanistic basis for preferential deadenylation of U6 snRNA by Usb1. *Nucleic Acids Research*, **2018**, 46, 11488-11501	20.1	9
108	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	4.6	16
107	Microscopic mechanisms that govern the titration response and pK values of buried residues in staphylococcal nuclease mutants. *Proteins: Structure, Function and Bioinformatics*, **2017**, 85, 268-281	4.2	22
106	Regulation and Plasticity of Catalysis in Enzymes: Insights from Analysis of Mechanochemical Coupling in Myosin. *Biochemistry*, **2017**, 56, 1482-1497	3.2	27
105	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	3.8	12
104	Intermolecular interactions in the condensed phase: Evaluation of semi-empirical quantum mechanical methods. *Journal of Chemical Physics*, **2017**, 147, 161704	3.9	7
103	Quantifying the Electrostatics of Polycation-Lipid Bilayer Interactions. *Journal of the American Chemical Society*, **2017**, 139, 5808-5816	16.4	29
102	Cavity hydration dynamics in cytochrome oxidase and functional implications. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E8830-E8836	11.5	19
101	Benchmarking density functional tight binding models for barrier heights and reaction energetics of organic molecules. *Journal of Computational Chemistry*, **2017**, 38, 2171-2185	3.5	25
100	Cover Image, Volume 85, Issue 2. *Proteins: Structure, Function and Bioinformatics*, **2017**, 85, C4-C4	4.2	
99	Substrate and Transition State Binding in Alkaline Phosphatase Analyzed by Computation of Oxygen Isotope Effects. *Journal of the American Chemical Society*, **2016**, 138, 11946-57	16.4	24
98	Sustainable Nanotechnology: Opportunities and Challenges for Theoretical/Computational Studies. *Journal of Physical Chemistry B*, **2016**, 120, 7297-306	3.4	42
97	Different states of synaptotagmin regulate evoked versus spontaneous release. *Nature Communications*, **2016**, 7, 10971	17.4	32
96	Gating mechanism of mechanosensitive channel of large conductance: a coupled continuum mechanical-continuum solvation approach. *Biomechanics and Modeling in Mechanobiology*, **2016**, 15, 1557-1576	3.8	10

95	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, 8424-37	3.4	17
94	A computational investigation on the substrate preference of ten-eleven-translocation 2 (TET2). *Physical Chemistry Chemical Physics*, **2016**, 18, 4728-38	3.6	16
93	Copper Oxidation/Reduction in Water and Protein: Studies with DFTB3/MM and VALBOND Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2016**, 120, 1894-910	3.4	19
92	First-Principles United Atom Force Field for the Ionic Liquid BMIM(+)BF4(-): An Alternative to Charge Scaling. *Journal of Physical Chemistry B*, **2016**, 120, 3560-8	3.4	52
91	Structure and dynamics underlying elementary ligand binding events in human pacemaking channels. *ELife*, **2016**, 5,	8.9	30
90	Towards a barrier height benchmark set for biologically relevant systems. *PeerJ*, **2016**, 4, e1994	3.1	15
89	Comparison of native and non-native ubiquitin oligomers reveals analogous structures and reactivities. *Protein Science*, **2016**, 25, 456-71	6.3	12
88	Predicting the Structure-Activity Relationship of Hydroxyapatite-Binding Peptides by Enhanced-Sampling Molecular Simulation. *Langmuir*, **2016**, 32, 7009-22	4	35
87	QM/MM free energy simulations: recent progress and challenges. *Molecular Simulation*, **2016**, 42, 1056-1078	2	63
86	Perspective: Quantum mechanical methods in biochemistry and biophysics. *Journal of Chemical Physics*, **2016**, 145, 140901	3.9	54
85	A composite approach towards a complete model of the myosin rod. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 172-189	4.2	8
84	Leaving Group Ability Observably Affects Transition State Structure in a Single Enzyme Active Site. *Journal of the American Chemical Society*, **2016**, 138, 7386-94	16.4	32
83	Semiempirical Quantum Mechanical Methods for Noncovalent Interactions for Chemical and Biochemical Applications. *Chemical Reviews*, **2016**, 116, 5301-37	68.1	210
82	Multiple gas-phase conformations of proline-containing peptides: is it always cis/trans isomerization?. *Analyst, The*, **2016**, 141, 4863-9	5	5
81	Interplay of Electrostatics and Hydrophobic Effects in the Metamorphic Protein Human Lymphotactin. *Journal of Physical Chemistry B*, **2015**, 119, 9547-58	3.4	1
80	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	11.5	34
79	The histone H3 N-terminal tail: a computational analysis of the free energy landscape and kinetics. *Physical Chemistry Chemical Physics*, **2015**, 17, 13689-98	3.6	8
78	Quantum effects in cation interactions with first and second coordination shell ligands in metalloproteins. *Journal of Chemical Theory and Computation*, **2015**, 11, 4992-5001	6.4	36

77	Structural insight into substrate preference for TET-mediated oxidation. *Nature*, **2015**, 527, 118-22	50.4	159
76	Anionic Phospholipids Stabilize RecA Filament Bundles in Escherichia coli. *Molecular Cell*, **2015**, 60, 374-84	17.6	36
75	DFTB3 Parametrization for Copper: The Importance of Orbital Angular Momentum Dependence of Hubbard Parameters. *Journal of Chemical Theory and Computation*, **2015**, 11, 4205-19	6.4	27
74	Molecular mechanisms for intrafibrillar collagen mineralization in skeletal tissues. *Biomaterials*, **2015**, 39, 59-66	15.6	72
73	Microscopic basis for kinetic gating in Cytochrome c oxidase: insights from QM/MM analysis. *Chemical Science*, **2015**, 6, 826-841	9.4	30
72	Parametrization of DFTB3/3OB for magnesium and zinc for chemical and biological applications. *Journal of Physical Chemistry B*, **2015**, 119, 1062-82	3.4	90
71	Improving intermolecular interactions in DFTB3 using extended polarization from chemical-potential equalization. *Journal of Chemical Physics*, **2015**, 143, 084123	3.9	38
70	Biological Responses to Engineered Nanomaterials: Needs for the Next Decade. *ACS Central Science*, **2015**, 1, 117-23	16.8	93
69	Parameterization of DFTB3/3OB for Sulfur and Phosphorus for Chemical and Biological Applications. *Journal of Chemical Theory and Computation*, **2014**, 10, 1518-1537	6.4	195
68	Quantum mechanical/molecular mechanical studies of zinc hydrolases. *International Reviews in Physical Chemistry*, **2014**, 33, 1-41	7	19
67	Molecular simulation of water and hydration effects in different environments: challenges and developments for DFTB based models. *Journal of Physical Chemistry B*, **2014**, 118, 11007-27	3.4	74
66	Small molecule-mediated control of hydroxyapatite growth: free energy calculations benchmarked to density functional theory. *Journal of Computational Chemistry*, **2014**, 35, 70-81	3.5	39
65	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, 2845-59	6.4	19
64	Density functional tight binding: values of semi-empirical methods in an ab initio era. *Physical Chemistry Chemical Physics*, **2014**, 16, 14368-77	3.6	98
63	Structural analysis and modeling reveals new mechanisms governing ESCRT-III spiral filament assembly. *Journal of Cell Biology*, **2014**, 206, 763-77	7.3	92
62	Density functional tight binding: application to organic and biological molecules. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2014**, 4, 49-61	7.9	127
61	Infrared spectral marker bands characterizing a transient water wire inside a hydrophobic membrane protein. *Journal of Chemical Physics*, **2014**, 141, 22D524	3.9	34
60	Tethered spectroscopic probes estimate dynamic distances with subnanometer resolution in voltage-dependent potassium channels. *Biophysical Journal*, **2013**, 105, 2724-32	2.9	9

59	A comparison of coarse-grained and continuum models for membrane bending in lipid bilayer fusion pores. *Biophysical Journal*, **2013**, 104, 841-52	2.9	23
58	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, 5059-69	6.4	28
57	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, 18886-91	11.5	45
56	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, 2005-18	3.4	26
55	Why do arginine and lysine organize lipids differently? Insights from coarse-grained and atomistic simulations. *Journal of Physical Chemistry B*, **2013**, 117, 12145-56	3.4	52
54	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, 10457-69	16.4	77
53	Generation and sensing of membrane curvature: Where materials science and biophysics meet. *Current Opinion in Solid State and Materials Science*, **2013**, 17, 164-174	12	19
52	Allosteric activation transitions in enzymes and biomolecular motors: insights from atomistic and coarse-grained simulations. *Topics in Current Chemistry*, **2013**, 337, 139-64		11
51	Three-dimensional stress field around a membrane protein: atomistic and coarse-grained simulation analysis of gramicidin A. *Biophysical Journal*, **2013**, 104, 117-27	2.9	24
50	Toward molecular models of proton pumping: Challenges, methods and relevant applications. *Science China Chemistry*, **2012**, 55, 3-18	7.9	6
49	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, 229-46	16.4	66
48	Detailed structure of the H2PO4(-)-guanosine diphosphate intermediate in Ras-GAP decoded from FTIR experiments by biomolecular simulations. *Journal of the American Chemical Society*, **2012**, 134, 20041-4	16.4	28
47	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	2.3	26
46	DFTB3: Extension of the self-consistent-charge density-functional tight-binding method (SCC-DFTB). *Journal of Chemical Theory and Computation*, **2012**, 7, 931-948	6.4	620
45	A New Coarse-Grained Force Field for Membrane-Peptide Simulations. *Journal of Chemical Theory and Computation*, **2011**, 7, 3793-802	6.4	70
44	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, 14981-97	16.4	48
43	Application of the SCC-DFTB method to neutral and protonated water clusters and bulk water. *Journal of Physical Chemistry B*, **2011**, 115, 6790-805	3.4	71
42	Interconversion of functional motions between mesophilic and thermophilic adenylate kinases. *PLoS Computational Biology*, **2011**, 7, e1002103	5	18

41	A new coarse-grained model for water: the importance of electrostatic interactions. *Journal of Physical Chemistry B*, **2010**, 114, 10524-9	3.4	150
40	An implicit solvent model for SCC-DFTB with Charge-Dependent Radii. *Journal of Chemical Theory and Computation*, **2010**, 6, 2303-2314	6.4	30
39	Self-Assembly of β-Peptides: Insight from the Pair and Many-Body Free Energy of Association. *Journal of Physical Chemistry C*, **2010**, 114, 13551-13556	3.8	11
38	Many local motions cooperate to produce the adenylate kinase conformational transition. *Journal of Molecular Biology*, **2010**, 400, 618-31	6.5	78
37	Proton transfer function of carbonic anhydrase: Insights from QM/MM simulations. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2010**, 1804, 342-51	4	48
36	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, 4930-9	3.4	28
35	Microscopic pKa analysis of Glu286 in cytochrome c oxidase (Rhodobacter sphaeroides): toward a calibrated molecular model. *Biochemistry*, **2009**, 48, 2468-85	3.2	53
34	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, 12439-46	2.8	42
33	Multi-Scale QM/MM Methods with Self-Consistent-Charge Density-Functional-Tight-Binding (SCC-DFTB). *Challenges and Advances in Computational Chemistry and Physics*, **2009**, 173-196	0.7	6
32	Allostery and cooperativity revisited. *Protein Science*, **2008**, 17, 1295-307	6.3	511
31	Extensive conformational transitions are required to turn on ATP hydrolysis in myosin. *Journal of Molecular Biology*, **2008**, 381, 1407-20	6.5	67
30	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	6.4	76
29	pKa of residue 66 in Staphylococal nuclease. I. Insights from QM/MM simulations with conventional sampling. *Journal of Physical Chemistry B*, **2008**, 112, 8387-97	3.4	45
28	Proton transfer in carbonic anhydrase is controlled by electrostatics rather than the orientation of the acceptor. *Biochemistry*, **2008**, 47, 2369-78	3.2	76
27	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, 19672-7	11.5	78
26	Extension of the self-consistent-charge density-functional tight-binding method: 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, 10861-73	2.8	221
25	Establishing Effective Simulation Protocols for β- and α/β-Mixed Peptides. I. QM and QM/MM Models. *Journal of Chemical Theory and Computation*, **2007**, 3, 1538-49	6.4	31
24	Specific Reaction Parametrization of the AM1/d Hamiltonian for Phosphoryl Transfer Reactions: H, O, and P Atoms. *Journal of Chemical Theory and Computation*, **2007**, 3, 486-504	6.4	131

23	Mechanochemical coupling in the myosin motor domain. I. Insights from equilibrium active-site simulations. *PLoS Computational Biology*, **2007**, 3, e21	5	41
22	pKa analysis for the zinc-bound water in human carbonic anhydrase II: Benchmark for "multiscale" QM/MM simulations and mechanistic implications. *Journal of Physical Chemistry A*, **2007**, 111, 5703-11	2.8	56
21	Development of effective quantum mechanical/molecular mechanical (QM/MM) methods for complex biological processes. *Journal of Physical Chemistry B*, **2006**, 110, 6458-69	3.4	274
20	"Proton holes" in long-range proton transfer reactions in solution and enzymes: A theoretical analysis. *Journal of the American Chemical Society*, **2006**, 128, 16302-11	16.4	111
19	pKa calculations in solution and proteins with QM/MM free energy perturbation simulations: a quantitative test of QM/MM protocols. *Journal of Physical Chemistry B*, **2005**, 109, 17715-33	3.4	145
18	Reliable treatment of electrostatics in combined QM/MM simulation of macromolecules. *Journal of Chemical Physics*, **2005**, 123, 014905	3.9	113
17	Mechanochemical Coupling in Myosin: A Theoretical Analysis with Molecular Dynamics and Combined QM/MM Reaction Path Calculations. *Journal of Physical Chemistry B*, **2004**, 108, 3342-3357	3.4	70
16	Importance of van der Waals Interactions in QM/MM Simulations. *Journal of Physical Chemistry B*, **2004**, 108, 6467-78	3.4	101
15	A normal mode analysis of structural plasticity in the biomolecular motor F(1)-ATPase. *Journal of Molecular Biology*, **2004**, 340, 345-72	6.5	142
14	Catalysis and specificity in enzymes: a study of triosephosphate isomerase and comparison with methyl glyoxal synthase. *Advances in Protein Chemistry*, **2003**, 66, 315-72		61
13	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, 565-81	3.5	146
12	Understanding the Role of Active-Site Residues in Chorismate Mutase Catalysis from Molecular-Dynamics Simulations. *Angewandte Chemie*, **2003**, 115, 1546-1549	3.6	2
11	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	3.4	101
10	A dynamic analysis of the rotation mechanism for conformational change in F(1)-ATPase. *Structure*, **2002**, 10, 921-31	5.2	147
9	Combining implicit solvation models with hybrid quantum mechanical/molecular mechanical methods: A critical test with glycine. *Journal of Chemical Physics*, **2002**, 117, 4720-4728	3.9	72
8	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	32
7	Quantum Mechanical/Molecular Mechanical Studies of the Triosephosphate Isomerase-Catalyzed Reaction: Verification of Methodology and Analysis of Reaction Mechanisms. *Journal of Physical Chemistry B*, **2002**, 106, 1768-1798	3.4	56
6	Quantum mechanics/molecular mechanics studies of triosephosphate isomerase-catalyzed reactions: effect of geometry and tunneling on proton-transfer rate constants. *Journal of the American Chemical Society*, **2002**, 124, 3093-124	16.4	114

5	Promoting Modes and Demoting Modes in Enzyme-Catalyzed Proton Transfer Reactions: A Study of Models and Realistic Systems. *Journal of Physical Chemistry B*, **2002**, 106, 7927-7947	3.4	70
4	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	3.4	523
3	Triosephosphate isomerase: a theoretical comparison of alternative pathways. *Journal of the American Chemical Society*, **2001**, 123, 2284-90	16.4	94
2	Molecular properties from combined QM/MM methods. I. Analytical second derivative and vibrational calculations. *Journal of Chemical Physics*, **2000**, 112, 1133-1149	3.9	137
1	Molecular Properties from Combined QM/MM Methods. 2. Chemical Shifts in Large Molecules. *Journal of Physical Chemistry B*, **2000**, 104, 3721-3743	3.4	132