

# Jiali Gao

## List of Publications by Year in descending order

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192  
papers

14,805  
citations

14614

66  
h-index

19690

117  
g-index

198  
all docs

198  
docs citations

198  
times ranked

9632  
citing authors

#	ARTICLE	IF	CITATIONS
1	Structural Basis for the Friedel-Crafts Alkylation in Cyclopropane Biosynthesis. ACS Catalysis, 2022, 12, 2108-2117.	5.5	7
2	Quantum vibration perturbation approach with polyatomic probe in simulating infrared spectra. Physical Chemistry Chemical Physics, 2022, 24, 1174-1182.	1.3	2
3	Dynamics and mechanism of dimer dissociation of photoreceptor UVR8. Nature Communications, 2022, 13, 93.	5.8	9
4	CARNOT: a Fragment-Based Direct Molecular Dynamics and Virtual Reality Simulation Package for Reactive Systems. Journal of Chemical Theory and Computation, 2022, 18, 1297-1313.	2.3	10
5	The Age of Direct Chemical Dynamics. Accounts of Chemical Research, 2022, 55, 471-472.	7.6	0
6	Origin of thiocyanate spectral shifts in water and organic solvents. Journal of Chemical Physics, 2022, 156, 104106.	1.2	6
7	Community Reaction Network Reduction for Constructing a Coarse-Grained Representation of Combustion Reaction Mechanisms. Journal of Chemical Information and Modeling, 2022, 62, 2352-2364.	2.5	6
8	Minimal Active Space for Diradicals Using Multistate Density Functional Theory. Molecules, 2022, 27, 3466.	1.7	1
9	Solvation Induction of Free Energy Barriers of Decarboxylation Reactions in Aqueous Solution from Dual-Level QM/MM Simulations. JACS Au, 2021, 1, 233-244.	3.6	8
10	SARS-CoV-2 spike protein N501Y mutation causes differential species transmissibility and antibody sensitivity: a molecular dynamics and alchemical free energy study. Molecular Systems Design and Engineering, 2021, 6, 964-974.	1.7	8
11	Conserved Conformational Hierarchy across Functionally Divergent Glycosyltransferases of the GT-B Structural Superfamily as Determined from Microsecond Molecular Dynamics. International Journal of Molecular Sciences, 2021, 22, 4619.	1.8	10
12	Activation mechanism of <i>Drosophila</i> cryptochrome through an allosteric switch. Science Advances, 2021, 7, .	4.7	14
13	Exact-two-component block-localized wave function: A simple scheme for the automatic computation of relativistic $\hat{T}^2$ SCF. Journal of Chemical Physics, 2021, 155, 014103.	1.2	5
14	Dynamic-then-Static Approach for Core Excitations of Open-Shell Molecules. Journal of Physical Chemistry Letters, 2021, 12, 7409-7417.	2.1	19
15	Variational Energy Decomposition Analysis of Charge-Transfer Interactions between Metals and Ligands in Carbonyl Complexes. Inorganic Chemistry, 2021, 60, 14060-14071.	1.9	5
16	Is Disrupted Nucleotide-Substrate Cooperativity a Common Trait for Cushing's Syndrome Driving Mutations of Protein Kinase A?. Journal of Molecular Biology, 2021, 433, 167123.	2.0	8
17	Minimal-active-space multistate density functional theory for excitation energy involving local and charge transfer states. Npj Computational Materials, 2021, 7, .	3.5	12
18	Block-Localized Excitation for Excimer Complex and Diabatic Coupling. Journal of Chemical Theory and Computation, 2021, 17, 240-254.	2.3	18

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19	Generalization of Block-Localized Wave Function for Constrained Optimization of Excited Determinants. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 277-289.	2.3	18
20	Origin of Free Energy Barriers of Decarboxylation and the Reverse Process of CO <sub>2</sub> Capture in Dimethylformamide and in Water. <i>Journal of the American Chemical Society</i> , 2021, 143, 137-141.	6.6	16
21	Deuterium Isotope Effects on Acid-Base Equilibrium of Organic Compounds. <i>Molecules</i> , 2021, 26, 7687.	1.7	1
22	Intrinsically disordered HAX-1 regulates Ca <sup>2+</sup> cycling by interacting with lipid membranes and the phospholamban cytoplasmic region. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2020, 1862, 183034.	1.4	8
23	Source code, input data, and sample output concerning the application of multistate density functional theory to the singdoublet and tripdoublet states of the ethylene cation. <i>Data in Brief</i> , 2020, 28, 104984.	0.5	1
24	Coupled electron and proton transfer in the piperidine drug metabolism pathway by the active species of cytochromes P450. <i>Dalton Transactions</i> , 2020, 49, 11099-11107.	1.6	4
25	Dynamics and mechanism of light harvesting in UV photoreceptor UVR8. <i>Chemical Science</i> , 2020, 11, 12553-12569.	3.7	3
26	A leap in quantum efficiency through light harvesting in photoreceptor UVR8. <i>Nature Communications</i> , 2020, 11, 4316.	5.8	20
27	Exploring the Reaction Mechanism of HIV Reverse Transcriptase with a Nucleotide Substrate. <i>Journal of Physical Chemistry B</i> , 2020, 124, 4270-4283.	1.2	7
28	A self-consistent coulomb bath model using density fitting. <i>Journal of Computational Chemistry</i> , 2020, 41, 1698-1708.	1.5	6
29	Enhanced receptor binding of SARS-CoV-2 through networks of hydrogen-bonding and hydrophobic interactions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 13967-13974.	3.3	291
30	Dynamical and allosteric regulation of photoprotection in light harvesting complex II. <i>Science China Chemistry</i> , 2020, 63, 1121-1133.	4.2	29
31	Fragment Exchange Potential for Realizing Pauli Deformation of Interfragment Interactions. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 4008-4016.	2.1	13
32	Sunitinib inhibits RNase L by destabilizing its active dimer conformation. <i>Biochemical Journal</i> , 2020, 477, 3387-3399.	1.7	10
33	Multi-state recognition pathway of the intrinsically disordered protein kinase inhibitor by protein kinase A. <i>ELife</i> , 2020, 9, .	2.8	16
34	Multistate density functional theory applied with 3 unpaired electrons in 3 orbitals: The singdoublet and tripdoublet states of the ethylene cation. <i>Chemical Physics Letters</i> , 2019, 736, 136803.	1.2	19
35	Cushing's syndrome driver mutation disrupts protein kinase A allosteric network, altering both regulation and substrate specificity. <i>Science Advances</i> , 2019, 5, eaaw9298.	4.7	43
36	What factors tune the chemical equilibrium between metal-iodosylarene oxidants and high-valent metal-oxo ones?. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 1271-1276.	1.3	6

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37	Catalytic hydrogen atom transfer from hydrosilanes to vinylarenes for hydrosilylation and polymerization. <i>Nature Catalysis</i> , 2019, 2, 164-173.	16.1	33
38	Why Can Normal Palladium Catalysts Efficiently Mediate Aerobic C-H Hydroxylation of Arylpyridines by Intercepting Aldehyde Autoxidation? A Nascent Palladium(III) Peracid Intermediate Makes a Difference. <i>Inorganic Chemistry</i> , 2019, 58, 4376-4384.	1.9	7
39	Active-Site Heterogeneity of Lactate Dehydrogenase. <i>ACS Catalysis</i> , 2019, 9, 4236-4246.	5.5	10
40	Molecular-bond breaking induced by interatomic decay processes. <i>Physical Review A</i> , 2019, 100, .	1.0	2
41	Conformational Landscape of the PRKACA-DNAJB1 Chimeric Kinase, the Driver for Fibrolamellar Hepatocellular Carcinoma. <i>Scientific Reports</i> , 2018, 8, 720.	1.6	23
42	Comment on "Substrate Folding Modes in Trichodiene Synthase: A Determinant of Chemo- and Stereoselectivity". <i>ACS Catalysis</i> , 2018, 8, 1371-1375.	5.5	17
43	The charger transfer electronic coupling in diabatic perspective: A multi-state density functional theory study. <i>Chemical Physics Letters</i> , 2018, 691, 91-97.	1.2	11
44	Dual QM and MM Approach for Computing Equilibrium Isotope Fractionation Factor of Organic Species in Solution. <i>Molecules</i> , 2018, 23, 2644.	1.7	3
45	Diabatic States at Construction (DAC) through Generalized Singular Value Decomposition. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 6038-6046.	2.1	13
46	Probing Protein-Protein Interactions Using Asymmetric Labeling and Carbonyl-Carbon Selective Heteronuclear NMR Spectroscopy. <i>Molecules</i> , 2018, 23, 1937.	1.7	9
47	Combined Multistate and Kohn-Sham Density Functional Theory Studies of the Elusive Mechanism of N-Dealkylation of N,N-Dimethylanilines Mediated by the Biomimetic Nonheme Oxidant FeIV(O)(N4Py)(ClO4)2. <i>Frontiers in Chemistry</i> , 2018, 6, 406.	1.8	7
48	The Stories Tryptophans Tell: Exploring Protein Dynamics of Heptosyltransferase I from <i>Escherichia coli</i> . <i>Biochemistry</i> , 2017, 56, 886-895.	1.2	20
49	Diabatic-At-Construction Method for Diabatic and Adiabatic Ground and Excited States Based on Multistate Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1176-1187.	2.3	49
50	Chemical Control in the Battle against Fidelity in Promiscuous Natural Product Biosynthesis: The Case of Trichodiene Synthase. <i>ACS Catalysis</i> , 2017, 7, 812-818.	5.5	48
51	Enhanced vibrational solvatochromism and spectral diffusion by electron rich substituents on small molecule silanes. <i>Journal of Chemical Physics</i> , 2017, 147, 124302.	1.2	10
52	Spin-Multiplet Components and Energy Splittings by Multistate Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4838-4845.	2.1	37
53	Perturbation Approach for Computing Infrared Spectra of the Local Mode of Probe Molecules. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 191-201.	2.3	10
54	Oxidation increases the strength of the methionine-aromatic interaction. <i>Nature Chemical Biology</i> , 2016, 12, 860-866.	3.9	53

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55	Beyond Kohn-Sham Approximation: Hybrid Multistate Wave Function and Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 5143-5149.	2.1	66
56	Multistate Density Functional Theory for Effective Diabatic Electronic Coupling. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2286-2293.	2.1	59
57	Two Aromatic Rings Coupled a Sulfur-Containing Group to Favor Protein Electron Transfer by Instantaneous Formations of $\pi$ -Sulfur or $\pi$ -Sulfur Five-Electron Bindings. <i>Journal of Physical Chemistry C</i> , 2015, 119, 9149-9158.	1.5	7
58	Dysfunctional conformational dynamics of protein kinase A induced by a lethal mutant of phospholamban hinder phosphorylation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 3716-3721.	3.3	43
59	Quantum mechanical force field for hydrogen fluoride with explicit electronic polarization. <i>Journal of Chemical Physics</i> , 2014, 140, 204501.	1.2	10
60	NMR mapping of protein conformational landscapes using coordinated behavior of chemical shifts upon ligand binding. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 6508-6518.	1.3	54
61	Investigating the role of a backbone to substrate hydrogen bond in OMP decarboxylase using a site-specific amide to ester substitution. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 15066-15071.	3.3	15
62	QM/MM through the 1990s: The First Twenty Years of Method Development and Applications. <i>Israel Journal of Chemistry</i> , 2014, 54, 1250-1263.	1.0	45
63	Explicit Polarization: A Quantum Mechanical Framework for Developing Next Generation Force Fields. <i>Accounts of Chemical Research</i> , 2014, 47, 2837-2845.	7.6	82
64	Beyond QM/MM: Fragment Quantum Mechanical Methods. <i>Accounts of Chemical Research</i> , 2014, 47, 2711-2711.	7.6	14
65	AM1/d-CB1: A Semiempirical Model for QM/MM Simulations of Chemical Glycobiology Systems. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4694-4707.	2.3	32
66	Quantum mechanical force field for water with explicit electronic polarization. <i>Journal of Chemical Physics</i> , 2013, 139, 054503.	1.2	36
67	The Quantum Coherent Mechanism for Singlet Fission: Experiment and Theory. <i>Accounts of Chemical Research</i> , 2013, 46, 1321-1329.	7.6	262
68	Communication: Variational many-body expansion: Accounting for exchange repulsion, charge delocalization, and dispersion in the fragment-based explicit polarization method. <i>Journal of Chemical Physics</i> , 2012, 136, 071101.	1.2	30
69	Fragment-based quantum mechanical methods for periodic systems with Ewald summation and mean image charge convention for long-range electrostatic interactions. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 7821.	1.3	23
70	Multilevel X-Pol: A Fragment-Based Method with Mixed Quantum Mechanical Representations of Different Fragments. <i>Journal of Physical Chemistry B</i> , 2012, 116, 6781-6788.	1.2	32
71	The Third Dimension of a More O <sup>2</sup> Ferrall-Jencks Diagram for Hydrogen Atom Transfer in the Isoelectronic Hydrogen Exchange Reactions of (PhX) <sub>2</sub> H <sup>+</sup> with X = O, NH, and CH <sub>2</sub> . <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4347-4358.	2.3	30
72	The Methionine-aromatic Motif Plays a Unique Role in Stabilizing Protein Structure. <i>Journal of Biological Chemistry</i> , 2012, 287, 34979-34991.	1.6	261

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73	Optimization of the explicit polarization (X-Pol) potential using a hybrid density functional. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1161.	0.5	15
74	Polarized Molecular Orbital Model Chemistry. 2. The PMO Method. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 857-867.	2.3	27
75	Kinetic Isotope Effects of $\text{L-Dopa}$ Decarboxylase. <i>Journal of the American Chemical Society</i> , 2011, 133, 4398-4403.	6.6	29
76	Energy decomposition analysis based on a block-localized wavefunction and multistate density functional theory. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 6760.	1.3	203
77	Incorporation of charge transfer into the explicit polarization fragment method by grand canonical density functional theory. <i>Journal of Chemical Physics</i> , 2011, 135, 084107.	1.2	16
78	Insight into the phosphodiesterase mechanism from combined QM/MM free energy simulations. <i>FEBS Journal</i> , 2011, 278, 2579-2595.	2.2	25
79	Using multipole point charge distributions to provide the electrostatic potential in the variational explicit polarization (X-Pol) potential. <i>Theoretical Chemistry Accounts</i> , 2011, 129, 3-13.	0.5	10
80	Computation of kinetic isotope effects for enzymatic reactions. <i>Science China Chemistry</i> , 2011, 54, 1841-1850.	4.2	8
81	The opsin shift and mechanism of spectral tuning in rhodopsin. <i>Journal of Computational Chemistry</i> , 2011, 32, 854-865.	1.5	44
82	Dipole preserving and polarization consistent charges. <i>Journal of Computational Chemistry</i> , 2011, 32, 2127-2139.	1.5	27
83	Dynamically committed, uncommitted, and quenched states encoded in protein kinase A revealed by NMR spectroscopy. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 6969-6974.	3.3	129
84	Generalized X-Pol Theory and Charge Delocalization States. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2402-2410.	2.3	26
85	A Non-Orthogonal Block-Localized Effective Hamiltonian Approach for Chemical and Enzymatic Reactions. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2242-2251.	2.3	18
86	On the Interfragment Exchange in the X-Pol Method. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2469-2476.	2.3	27
87	Internal Proton Transfer in the External Pyridoxal 5'-Phosphate Schiff Base in Dopa Decarboxylase. <i>Biochemistry</i> , 2010, 49, 84-94.	1.2	37
88	Differential quantum tunneling contributions in nitroalkane oxidase catalyzed and the uncatalyzed proton transfer reaction. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 20734-20739.	3.3	69
89	Block-Localized Density Functional Theory (BLDFT), Diabatic Coupling, and Their Use in Valence Bond Theory for Representing Reactive Potential Energy Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2702-2716.	2.3	110
90	A Coupled Polarization-Matrix Inversion and Iteration Approach for Accelerating the Dipole Convergence in a Polarizable Potential Function. <i>Journal of Physical Chemistry A</i> , 2009, 113, 2109-2116.	1.1	18

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91	An Effective Hamiltonian Molecular Orbital-Valence Bond (MOVB) Approach for Chemical Reactions as Applied to the Nucleophilic Substitution Reaction of Hydrosulfide Ion and Chloromethane. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 174-185.	2.3	22
92	Critical Role of Substrate Conformational Change in the Proton Transfer Process Catalyzed by 4-Oxalocrotonate Tautomerase. <i>Journal of the American Chemical Society</i> , 2009, 131, 2687-2698.	6.6	18
93	X-Pol Potential: An Electronic Structure-Based Force Field for Molecular Dynamics Simulation of a Solvated Protein in Water. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 459-467.	2.3	121
94	Perspective on Diabatic Models of Chemical Reactivity as Illustrated by the Gas-Phase SN2 Reaction of Acetate Ion with 1,2-Dichloroethane. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1-22.	2.3	45
95	Explicit Polarization (X-Pol) Potential Using ab Initio Molecular Orbital Theory and Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2009, 113, 11656-11664.	1.1	49
96	Combined QM/MM and path integral simulations of kinetic isotope effects in the proton transfer reaction between nitroethane and acetate ion in water. <i>Journal of Computational Chemistry</i> , 2008, 29, 514-522.	1.5	45
97	On the Construction of Diabatic and Adiabatic Potential Energy Surfaces Based on Ab Initio Valence Bond Theory. <i>Journal of Physical Chemistry A</i> , 2008, 112, 12925-12935.	1.1	59
98	Incorporation of a QM/MM Buffer Zone in the Variational Double Self-Consistent Field Method. <i>Journal of Physical Chemistry B</i> , 2008, 112, 14124-14131.	1.2	31
99	Molecular Dynamics Simulations of Biotin Carboxylase. <i>Journal of Physical Chemistry B</i> , 2008, 112, 3149-3156.	1.2	12
100	The variational explicit polarization potential and analytical first derivative of energy: Towards a next generation force field. <i>Journal of Chemical Physics</i> , 2008, 128, 234108.	1.2	104
101	Hybrid Quantum and Classical Methods for Computing Kinetic Isotope Effects of Chemical Reactions in Solutions and in Enzymes. <i>Methods in Molecular Biology</i> , 2008, 443, 37-62.	0.4	5
102	Methods and Applications of Combined Quantum Mechanical and Molecular Mechanical Potentials. <i>Reviews in Computational Chemistry</i> , 2007, , 119-185.	1.5	189
103	Theoretical Analysis of the Rotational Barrier of Ethane. <i>Accounts of Chemical Research</i> , 2007, 40, 113-119.	7.6	172
104	An Integrated Path Integral and Free-Energy Perturbation~Umbrella Sampling Method for Computing Kinetic Isotope Effects of Chemical Reactions in Solution and in Enzymes. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 949-960.	2.3	86
105	Development of a Polarizable Intermolecular Potential Function (PIPF) for Liquid Amides and Alkanes. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1878-1889.	2.3	107
106	Synthetic Efficiency in Enzyme Mechanisms Involving Carbocations:~Aristolochene Synthase. <i>Journal of the American Chemical Society</i> , 2007, 129, 13008-13013.	6.6	61
107	Design of a Next Generation Force Field:~The X-POL Potential. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1890-1900.	2.3	209
108	Specific Reaction Parametrization of the AM1/d Hamiltonian for Phosphoryl Transfer Reactions:~H, O, and P Atoms. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 486-504.	2.3	138



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109	Solvatochromic Shifts of the n $\rightarrow$ $\pi^*$ Transition of Acetone from Steam Vapor to Ambient Aqueous Solution: A Combined Configuration Interaction QM/MM Simulation Study Incorporating Solvent Polarization. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1484-1493.	2.3	53
110	Molecular Dynamics Simulations of the Catalytic Pathway of a Cysteine Protease: A Combined QM/MM Study of Human Cathepsin K. <i>Journal of the American Chemical Society</i> , 2007, 129, 13633-13645.	6.6	82
111	The Reaction Mechanism of Paraoxon Hydrolysis by Phosphotriesterase from Combined QM/MM Simulations. <i>Biochemistry</i> , 2007, 46, 13352-13369.	1.2	137
112	Potential energy functions for an intramolecular proton transfer reaction in the ground and excited state. <i>Theoretical Chemistry Accounts</i> , 2007, 118, 211-218.	0.5	8
113	Multidimensional Tunneling, Recrossing, and the Transmission Coefficient for Enzymatic Reactions. <i>Chemical Reviews</i> , 2006, 106, 3140-3169.	23.0	328
114	Mechanisms and Free Energies of Enzymatic Reactions. <i>Chemical Reviews</i> , 2006, 106, 3188-3209.	23.0	355
115	Path Integral Simulations of Proton Transfer Reactions in Aqueous Solution Using Combined QM/MM Potentials. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 236-245.	2.3	57
116	A Combined Quantum Mechanical and Molecular Mechanical Study of the Reaction Mechanism and $\Delta$ -Amino Acidity in Alanine Racemase. <i>Journal of the American Chemical Society</i> , 2006, 128, 16345-16357.	6.6	125
117	Implementation of the bisection sampling method in path integral simulations. <i>Journal of Molecular Graphics and Modelling</i> , 2005, 24, 121-127.	1.3	54
118	An Efficient Linear-Scaling Ewald Method for Long-Range Electrostatic Interactions in Combined QM/MM Calculations. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 2-13.	2.3	258
119	Solvent Polarization and Kinetic Isotope Effects in Nitroethane Deprotonation and Implications to the Nitroalkane Oxidase Reaction. <i>Journal of the American Chemical Society</i> , 2005, 127, 16374-16375.	6.6	50
120	Solvent and Protein Effects on the Vibrational Frequency Shift and Energy Relaxation of the Azide Ligand in Carbonic Anhydrase. <i>Journal of Physical Chemistry B</i> , 2004, 108, 13501-13512.	1.2	34
121	Generalized hybrid orbital for the treatment of boundary atoms in combined quantum mechanical and molecular mechanical calculations using the semiempirical parameterized model 3 method. <i>Theoretical Chemistry Accounts</i> , 2004, 111, 280-286.	0.5	35
122	Ensemble-averaged variational transition state theory with optimized multidimensional tunneling for enzyme kinetics and other condensed-phase reactions. <i>International Journal of Quantum Chemistry</i> , 2004, 100, 1136-1152.	1.0	122
123	The Magnitude of Hyperconjugation in Ethane: A Perspective from Ab Initio Valence Bond Theory. <i>Angewandte Chemie - International Edition</i> , 2004, 43, 1986-1990.	7.2	139
124	Combining Self-Consistent-Charge Density-Functional Tight-Binding (SCC-DFTB) with Molecular Mechanics by the Generalized Hybrid Orbital (GHO) Method. <i>Journal of Physical Chemistry A</i> , 2004, 108, 5454-5463.	1.1	94
125	How Enzymes Work: Analysis by Modern Rate Theory and Computer Simulations. <i>Science</i> , 2004, 303, 186-195.	6.0	1,048
126	Catalysis by enzyme conformational change as illustrated by orotidine 5 $\alpha$ -monophosphate decarboxylase. <i>Current Opinion in Structural Biology</i> , 2003, 13, 184-192.	2.6	58



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127	Balancing Kinetic and Thermodynamic Control: The Mechanism of Carbocation Cyclization by Squalene Cyclase. <i>Journal of the American Chemical Society</i> , 2003, 125, 12768-12781.	6.6	91
128	Perturbation Approach to Combined QM/MM Simulation of Solute-Solvent Interactions in Solution. <i>Journal of Physical Chemistry B</i> , 2003, 107, 1664-1671.	1.2	30
129	Combined QM/MM Study of the Mechanism and Kinetic Isotope Effect of the Nucleophilic Substitution Reaction in Haloalkane Dehalogenase. <i>Journal of the American Chemical Society</i> , 2003, 125, 1532-1540.	6.6	75
130	Free Energy Surface, Reaction Paths, and Kinetic Isotope Effect of Short-Chain Acyl-CoA Dehydrogenase. <i>Journal of Physical Chemistry B</i> , 2003, 107, 9567-9578.	1.2	75
131	Importance of Electronic Delocalization on the C-N Bond Rotation in HCX(NH <sub>2</sub> ) (X = O, NH, CH <sub>2</sub> , S, and Tj ETQq 1.1 0.784314 rgBT 59)	1.1	59
132	Reaction-Path Energetics and Kinetics of the Hydride Transfer Reaction Catalyzed by Dihydrofolate Reductase. <i>Biochemistry</i> , 2003, 42, 13558-13575.	1.2	202
133	Importance of Substrate and Cofactor Polarization in the Active Site of Dihydrofolate Reductase. <i>Journal of Molecular Biology</i> , 2003, 327, 549-560.	2.0	78
134	Hydrogen fluoride phase behavior and molecular structure: A QM/MM potential model approach. <i>Journal of Chemical Physics</i> , 2003, 119, 7365-7371.	1.2	26
135	The Incorporation of Quantum Effects in Enzyme Kinetics Modeling. <i>Accounts of Chemical Research</i> , 2002, 35, 341-349.	7.6	240
136	QUANTUMMECHANICALMETHODS FORENZYMEKINETICS. <i>Annual Review of Physical Chemistry</i> , 2002, 53, 467-505.	4.8	730
137	Cation- $\pi$ Interactions: An Energy Decomposition Analysis and Its Implication in $\mu$ -Opioid Receptor-Ligand Binding. <i>Journal of the American Chemical Society</i> , 2002, 124, 4832-4837.	6.6	131
138	Combined QM/MM study of the opsin shift in bacteriorhodopsin. <i>Journal of Computational Chemistry</i> , 2002, 23, 96-105.	1.5	81
139	Polarization and Charge-Transfer Effects in Lewis Acid-Base Complexes. <i>Journal of Physical Chemistry A</i> , 2001, 105, 6530-6536.	1.1	87
140	Canonical Variational Theory for Enzyme Kinetics with the Protein Mean Force and Multidimensional Quantum Mechanical Tunneling Dynamics. Theory and Application to Liver Alcohol Dehydrogenase. <i>Journal of Physical Chemistry B</i> , 2001, 105, 11326-11340.	1.2	184
141	Inclusion of quantum-mechanical vibrational energy in reactive potentials of mean force. <i>Journal of Chemical Physics</i> , 2001, 114, 9953-9958.	1.2	84
142	Hydrogen-bonding interactions in the active site of a low molecular weight protein-tyrosine phosphatase. <i>Journal of Computational Chemistry</i> , 2000, 21, 1192-1203.	1.5	16
143	Ab initio QM/MM simulations with a molecular orbital-valence bond (MOVb) method: application to an S <sub>N</sub> 2 reaction in water. <i>Journal of Computational Chemistry</i> , 2000, 21, 1458-1469.	1.5	146
144	The generalized hybrid orbital method for combined quantum mechanical/molecular mechanical calculations: formulation and tests of the analytical derivatives. <i>Theoretical Chemistry Accounts</i> , 2000, 104, 336-343.	0.5	110

#	ARTICLE	IF	CITATIONS
145	Perspective on "Theoretical studies of enzymic reactions: dielectric, electrostatic and steric stabilization of the carbonium ion in the reaction of lysozyme". <i>Theoretical Chemistry Accounts</i> , 2000, 103, 328-329.	0.5	3
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