Yingkai Zhang

List of Publications by Year
in descending order

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115 papers	9,625 citations	57758 44 h-index	37204 96 g-index
117 all docs	117 docs citations	117 times ranked	9340 citing authors

#	Article	IF	Citations
1	Comment on â€œGeneralized Gradient Approximation Made Simpleâ€. Physical Review Letters, 1998, 80, 890-890.	7.8	2,323
2	A challenge for density functionals: Self-interaction error increases for systems with a noninteger number of electrons. Journal of Chemical Physics, 1998, 109, 2604-2608.	3.0	524
3	A pseudobond approach to combining quantum mechanical and molecular mechanical methods. Journal of Chemical Physics, 1999, 110, 46-54.	3.0	460
4	Free energy calculation on enzyme reactions with an efficient iterative procedure to determine minimum energy paths on a combinedab initioQM/MM potential energy surface. Journal of Chemical Physics, 2000, 112, 3483-3492.	3.0	434
5	Degenerate Ground States and a Fractional Number of Electrons in Density and Reduced Density Matrix Functional Theory. Physical Review Letters, 2000, 84, 5172-5175.	7.8	390
6	Describing van der Waals Interaction in diatomic molecules with generalized gradient approximations: The role of the exchange functional. Journal of Chemical Physics, 1997, 107, 7921-7925.	3.0	282
7	Role of the Catalytic Triad and Oxyanion Hole in Acetylcholinesterase Catalysis:â€‰ An ab initio QM/MM Study. Journal of the American Chemical Society, 2002, 124, 10572-10577.	13.7	243
8	Improving scoring-docking-screening powers of protein-ligand scoring functions using random forest. Journal of Computational Chemistry, 2017, 38, 169-177.	3.3	201
9	Reaction Mechanism of Monoethanolamine with CO₂ in Aqueous Solution from Molecular Modeling. Journal of Physical Chemistry A, 2010, 114, 11844-11852.	2.5	161
10	Pseudobond ab initio QM/MM approach and its applications to enzyme reactions. Theoretical Chemistry Accounts, 2006, 116, 43-50.	1.4	148
11	Improved pseudobonds for combined ab initio quantum mechanical/molecular mechanical methods. Journal of Chemical Physics, 2005, 122, 024114.	3.0	147
12	Catalytic Mechanism and Product Specificity of the Histone Lysine Methyltransferase SET7/9:Â An ab Initio QM/MM-FE Study with Multiple Initial Structures. Journal of the American Chemical Society, 2006, 128, 1272-1278.	13.7	141
13	How Does the cAMP-Dependent Protein Kinase Catalyze the Phosphorylation Reaction:Â An ab Initio QM/MM Study. Journal of the American Chemical Society, 2005, 127, 1553-1562.	13.7	140
14	Density-based energy decomposition analysis for intermolecular interactions with variationally determined intermediate state energies. Journal of Chemical Physics, 2009, 131, 164112.	3.0	125
15	Perspective on "Density-functional theory for fractional particle number: derivative discontinuities of the energy". Theoretical Chemistry Accounts, 2000, 103, 346-348.	1.4	124
16	A Proton-Shuttle Reaction Mechanism for Histone Deacetylase 8 and the Catalytic Role of Metal Ions. Journal of the American Chemical Society, 2010, 132, 9471-9479.	13.7	121
17	A Water-Mediated and Substrate-Assisted Catalytic Mechanism forSulfolobus solfataricusDNA Polymerase IV. Journal of the American Chemical Society, 2007, 129, 4731-4737.	13.7	118
18	Catalytic Reaction Mechanism of Acetylcholinesterase Determined by Bornâ"Oppenheimer Ab Initio QM/MM Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 8817-8825.	2.6	109

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19	Influence of Structural Fluctuation on Enzyme Reaction Energy Barriers in Combined Quantum Mechanical/Molecular Mechanical Studies. Journal of Physical Chemistry B, 2003, 107, 4459-4463.	2.6	108
20	How Is the Active Site of Enolase Organized To Catalyze Two Different Reaction Steps?. Journal of the American Chemical Society, 2000, 122, 6560-6570.	13.7	103
21	Studying Enzyme Binding Specificity in Acetylcholinesterase Using a Combined Molecular Dynamics and Multiple Docking Approach. Journal of the American Chemical Society, 2002, 124, 8260-8267.	13.7	101
22	An efficient linear scaling method for ab initio calculation of electron density of proteins. Chemical Physics Letters, 2004, 394, 293-297.	2.6	100
23	Unexpected Deacetylation Mechanism Suggested by a Density Functional Theory QM/MM Study of Histone-Deacetylase-Like Protein. Journal of the American Chemical Society, 2006, 128, 4530-4531.	13.7	98
24	An efficient approach for ab initio energy calculation of biopolymers. Journal of Chemical Physics, 2005, 122, 184105.	3.0	96
25	Zinc Chelation with Hydroxamate in Histone Deacetylases Modulated by Water Access to the Linker Binding Channel. Journal of the American Chemical Society, 2011, 133, 6110-6113.	13.7	91
26	Ab Initio QM/MM Study Shows There Is No General Acid in the Reaction Catalyzed by 4-Oxalocrotonate Tautomerase. Journal of the American Chemical Society, 2003, 125, 10384-10393.	13.7	89
27	How Do SET-Domain Protein Lysine Methyltransferases Achieve the Methylation State Specificity? Revisited by Ab Initio QM/MM Molecular Dynamics Simulations. Journal of the American Chemical Society, 2008, 130, 3806-3813.	13.7	84
28	Ab Initio Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation of Enzyme Catalysis:â€‰ The Case of Histone Lysine Methyltransferase SET7/9. Journal of Physical Chemistry B, 2007, 111, 3758-3764.	2.6	78
29	Highly Dissociative and Concerted Mechanism for the Nicotinamide Cleavage Reaction in Sir2Tm Enzyme Suggested by Ab Initio QM/MM Molecular Dynamics Simulations. Journal of the American Chemical Society, 2008, 130, 16721-16728.	13.7	77
30	EGCG binds intrinsically disordered N-terminal domain of p53 and disrupts p53-MDM2 interaction. Nature Communications, 2021, 12, 986.	12.8	77
31	Flexibility of Catalytic Zinc Coordination in Thermolysin and HDAC8: A Bornâ"Oppenheimer ab Initio QM/MM Molecular Dynamics Study. Journal of Chemical Theory and Computation, 2010, 6, 337-343.	5.3	76
32	Targeting Amyloidogenic Processing of APP in Alzheimerâ€™s Disease. Frontiers in Molecular Neuroscience, 2020, 13, 137.	2.9	73
33	Resveratrol serves as a protein-substrate interaction stabilizer in human SIRT1 activation. Scientific Reports, 2016, 6, 38186.	3.3	71
34	Bimetallic Câ€“C Bond-Forming Reductive Elimination from Nickel. Journal of the American Chemical Society, 2016, 138, 4779-4786.	13.7	70
35	Interfacing ab Initio Quantum Mechanical Method with Classical Drude Osillator Polarizable Model for Molecular Dynamics Simulation of Chemical Reactions. Journal of Chemical Theory and Computation, 2008, 4, 1237-1248.	5.3	67
36	Mechanistic Insights into a Classic Wonder Drugâ€”Aspirin. Journal of the American Chemical Society, 2015, 137, 70-73.	13.7	66

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37	Incorporating Explicit Water Molecules and Ligand Conformation Stability in Machine-Learning Scoring Functions. Journal of Chemical Information and Modeling, 2019, 59, 4540-4549.	5.4	66
38	Molecular docking of balanol to dynamics snapshots of protein kinase A. Proteins: Structure, Function and Bioinformatics, 2005, 61, 850-858.	2.6	60
39	How does activation loop phosphorylation modulate catalytic activity in the cAMP-dependent protein kinase: A theoretical study. Protein Science, 2006, 15, 672-683.	7.6	55
40	Tuning the Membrane Selectivity of Antimicrobial Peptides by Using Multivalent Design. ChemBioChem, 2007, 8, 2063-2065.	2.6	55
41	Reaction Pathway and Free-Energy Barrier for Reactivation of Dimethylphosphoryl-Inhibited Human Acetylcholinesterase. Journal of Physical Chemistry B, 2009, 113, 16226-16236.	2.6	53
42	Aging Mechanism of Soman Inhibited Acetylcholinesterase. Journal of Physical Chemistry B, 2012, 116, 12199-12207.	2.6	51
43	Selective and noncovalent targeting of RAS mutants for inhibition and degradation. Nature Communications, 2021, 12, 2656.	12.8	51
44	Serine protease acylation proceeds with a subtle re-orientation of the histidine ring at the tetrahedral intermediate. Chemical Communications, 2011, 47, 1577-1579.	4.1	47
45	A Transferable Nonbonded Pairwise Force Field to Model Zinc Interactions in Metalloproteins. Journal of Chemical Theory and Computation, 2011, 7, 433-443.	5.3	47
46	AlphaSpace: Fragment-Centric Topographical Mapping To Target Proteinâ€“Protein Interaction Interfaces. Journal of Chemical Information and Modeling, 2015, 55, 1585-1599.	5.4	47
47	Studying the roles of W86, E202, and Y337 in binding of acetylcholine to acetylcholinesterase using a combined molecular dynamics and multiple docking approach. Protein Science, 2003, 12, 2675-2684.	7.6	41
48	Computational Design of a Time-Dependent Histone Deacetylase 2 Selective Inhibitor. ACS Chemical Biology, 2015, 10, 687-692.	3.4	41
49	Targeting Unoccupied Surfaces on Proteinâ€“Protein Interfaces. Journal of the American Chemical Society, 2017, 139, 15560-15563.	13.7	41
50	Bornâ^'Oppenheimer ab Initio QM/MM Molecular Dynamics Simulations of the Hydrolysis Reaction Catalyzed by Protein Arginine Deiminase 4. Journal of Physical Chemistry B, 2009, 113, 16705-16710.	2.6	37
51	Proteinâ€“Ligand Docking in the Machine-Learning Era. Molecules, 2022, 27, 4568.	3.8	37
52	Active Site Cysteine Is Protonated in the PAD4 Michaelis Complex: Evidence from Bornâ^'Oppenheimer Ab Initio QM/MM Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 12750-12758.	2.6	36
53	An Internal Water-Retention Site in the Rhomboid Intramembrane Protease GlpG Ensures Catalytic Efficiency. Structure, 2012, 20, 1255-1263.	3.3	36
54	Directional Dependence of Hydrogen Bonds: A Density-Based Energy Decomposition Analysis and Its Implications on Force Field Development. Journal of Chemical Theory and Computation, 2011, 7, 4038-4049.	5.3	35

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55	Design, synthesis and biological evaluation of quinoline derivatives as HDAC class I inhibitors. European Journal of Medicinal Chemistry, 2017, 133, 11-23.	5.5	35
56	Preferred WMSA catalytic mechanism of the nucleotidyl transfer reaction in human DNA polymerase Î¹ elucidates error-free bypass of a bulky DNA lesion. Nucleic Acids Research, 2012, 40, 9193-9205.	14.5	34
57	DNA Cytosine Methylation: Structural and Thermodynamic Characterization of the Epigenetic Marking Mechanism. Biochemistry, 2013, 52, 2828-2838.	2.5	33
58	Nucleotide Excision Repair Lesion-Recognition Protein Rad4 Captures a Pre-Flipped Partner Base in a Benzo[a]pyrene-Derived DNA Lesion: How Structure Impacts the Binding Pathway. Chemical Research in Toxicology, 2017, 30, 1344-1354.	3.3	32
59	Increasing the time step with mass scaling in Bornâ€Oppenheimer ab initio QM/MM molecular dynamics simulations. Journal of Computational Chemistry, 2009, 30, 2706-2711.	3.3	31
60	Molecular basis for receptor tyrosine kinase A-loop tyrosine transphosphorylation. Nature Chemical Biology, 2020, 16, 267-277.	8.0	31
61	Modulation of virus-induced NF-Î¹B signaling by NEMO coiled coil mimics. Nature Communications, 2020, 11, 1786.	12.8	30
62	Dominant role of CDKN2B/p15INK4B of 9p21.3 tumor suppressor hub in inhibition of cell-cycle and glycolysis. Nature Communications, 2021, 12, 2047.	12.8	30
63	Sirtuin Deacetylation Mechanism and Catalytic Role of the Dynamic Cofactor Binding Loop. Journal of Physical Chemistry Letters, 2013, 4, 491-495.	4.6	29
64	Polymerase-Tailored Variations in the Water-Mediated and Substrate-Assisted Mechanism for Nucleotidyl Transfer: Insights from a Study of T7 DNA Polymerase. Journal of Molecular Biology, 2009, 389, 787-796.	4.2	28
65	Molecular Mechanism for Eliminylation, a Newly Discovered Post-Translational Modification. Journal of the American Chemical Society, 2011, 133, 11103-11105.	13.7	28
66	Studying the affinity and kinetics of molecular association with molecular-dynamics simulation. Journal of Chemical Physics, 2003, 118, 1821-1827.	3.0	26
67	Catalytic Mechanism and Metal Specificity of Bacterial Peptide Deformylase:Â A Density Functional Theory QM/MM Study. Journal of Physical Chemistry B, 2007, 111, 6229-6235.	2.6	26
68	Side chain specificity of ADPâ€ribosylation by a sirtuin. FEBS Journal, 2009, 276, 7159-7176.	4.7	26
69	Base Flipping Free Energy Profiles for Damaged and Undamaged DNA. Chemical Research in Toxicology, 2010, 23, 1868-1870.	3.3	26
70	Recognition of Damaged DNA for Nucleotide Excision Repair: A Correlated Motion Mechanism with a Mismatched cis-syn Thymine Dimer Lesion. Biochemistry, 2015, 54, 5263-5267.	2.5	26
71	Delta Machine Learning to Improve Scoring-Ranking-Screening Performances of Proteinâ€“Ligand Scoring Functions. Journal of Chemical Information and Modeling, 2022, 62, 2696-2712.	5.4	26
72	Predicting Molecular Energy Using Force-Field Optimized Geometries and Atomic Vector Representations Learned from an Improved Deep Tensor Neural Network. Journal of Chemical Theory and Computation, 2019, 15, 4113-4121.	5.3	25

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73	How Is Acetylcholinesterase Phosphonylated by Soman? An Ab Initio QM/MM Molecular Dynamics Study. Journal of Physical Chemistry A, 2014, 118, 9132-9139.	2.5	24
74	Accurate Prediction of Aqueous Free Solvation Energies Using 3D Atomic Feature-Based Graph Neural Network with Transfer Learning. Journal of Chemical Information and Modeling, 2022, 62, 1840-1848.	5.4	24
75	QM/MM Molecular Dynamics Study of Purine-Specific Nucleoside Hydrolase. Journal of Physical Chemistry B, 2012, 116, 1984-1991.	2.6	23
76	Revelation of a Catalytic Calcium-Binding Site Elucidates Unusual Metal Dependence of a Human Apyrase. Journal of the American Chemical Society, 2012, 134, 15595-15603.	13.7	23
77	Bornâ€“Oppenheimer Ab Initio QM/MM Molecular Dynamics Simulations of Enzyme Reactions. Methods in Enzymology, 2016, 577, 105-118.	1.0	23
78	Importance of Charge Independent Effects in Readout of the Trimethyllysine Mark by HP1 Chromodomain. Journal of the American Chemical Society, 2009, 131, 14928-14931.	13.7	22
79	Ab Initio QM/MM Free-Energy Studies of Arginine Deiminase Catalysis: The Protonation State of the Cys Nucleophile. Journal of Physical Chemistry B, 2011, 115, 3725-3733.	2.6	22
80	Thiol versus hydroxamate as zinc binding group in <scp>HDAC</scp> inhibition: An Ab initio<scp>QM</scp>/<scp>MM</scp> molecular dynamics study. Journal of Computational Chemistry, 2015, 36, 2228-2235.	3.3	22
81	Design-atom approach for the quantum mechanical/molecular mechanical covalent boundary: A design-carbon atom with five valence electrons. Journal of Chemical Physics, 2007, 127, 124102.	3.0	20
82	Nucleosome Histone Tail Conformation and Dynamics: Impacts of Lysine Acetylation and a Nearby Minor Groove Benzo[a]pyrene-Derived Lesion. Biochemistry, 2017, 56, 1963-1973.	2.5	20
83	Lesion Sensing during Initial Binding by Yeast XPC/Rad4: Toward Predicting Resistance to Nucleotide Excision Repair. Chemical Research in Toxicology, 2018, 31, 1260-1268.	3.3	20
84	Peptide Conformation Analysis Using an Integrated Bayesian Approach. Journal of Chemical Theory and Computation, 2014, 10, 4152-4159.	5.3	19
85	Unified Deep Learning Model for Multitask Reaction Predictions with Explanation. Journal of Chemical Information and Modeling, 2022, 62, 1376-1387.	5.4	19
86	Free Energy Profiles of Base Flipping in Intercalative Polycyclic Aromatic Hydrocarbon-Damaged DNA Duplexes: Energetic and Structural Relationships to Nucleotide Excision Repair Susceptibility. Chemical Research in Toxicology, 2013, 26, 1115-1125.	3.3	18
87	Structural and Dynamic Characterization of Polymerase Îºâ€™s Minor Groove Lesion Processing Reveals How Adduct Topology Impacts Fidelity. Biochemistry, 2014, 53, 5683-5691.	2.5	16
88	A Conserved Allosteric Pathway in Tyrosine Kinase Regulation. Structure, 2019, 27, 1308-1315.e3.	3.3	16
89	Density functional study of a weakly hydrogen-bonded benzene-ammonia complex: The importance of the exchange functional. International Journal of Quantum Chemistry, 2000, 79, 325-329.	2.0	15
90	Geometric Preferences in Iron(II) and Zinc(II) Model Complexes of Peptide Deformylase. Inorganic Chemistry, 2006, 45, 1409-1411.	4.0	15

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91	Two symmetric arginine residues play distinct roles in Thermus thermophilus Argonaute DNA guide strand-mediated DNA target cleavage. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 845-853.	7.1	15
92	Perspective on â€œDensity-functional theory for fractional particle number: derivative discontinuities of the energyâ€•, 2000, , 346-348.		14
93	Intrinsic cleavage of RNA polymerase II adopts a nucleobase-independent mechanism assisted by transcript phosphate. Nature Catalysis, 2019, 2, 228-235.	34.4	13
94	Lin_F9: A Linear Empirical Scoring Function for Proteinâ€“Ligand Docking. Journal of Chemical Information and Modeling, 2021, 61, 4630-4644.	5.4	13
95	Peptide Tethering: Pocket-Directed Fragment Screening for Peptidomimetic Inhibitor Discovery. Journal of the American Chemical Society, 2022, 144, 1198-1204.	13.7	12
96	Dataset Construction to Explore Chemical Space with 3D Geometry and Deep Learning. Journal of Chemical Information and Modeling, 2021, 61, 1095-1104.	5.4	11
97	Determination of free energy profiles by repository based adaptive umbrella sampling: Bridging nonequilibrium and quasiequilibrium simulations. Journal of Chemical Physics, 2008, 128, 204106.	3.0	10
98	Entrapment of a Histone Tail by a DNA Lesion in a Nucleosome Suggests the Lesion Impacts Epigenetic Marking: A Molecular Dynamics Study. Biochemistry, 2016, 55, 239-242.	2.5	10
99	Synergistic effects of H3 and H4 nucleosome tails on structure and dynamics of a lesion-containing DNA: Binding of a displaced lesion partner base to the H3 tail for GG-NER recognition. DNA Repair, 2018, 65, 73-78.	2.8	10
100	Exploring fragment-based target-specific ranking protocol with machine learning on cathepsin S. Journal of Computer-Aided Molecular Design, 2019, 33, 1095-1105.	2.9	10
101	Improved parameterization of interatomic potentials for rare gas dimers with density-based energy decomposition analysis. Journal of Chemical Physics, 2014, 140, 214117.	3.0	8
102	Computational Strategy for Bound State Structure Prediction in Structure-Based Virtual Screening: A Case Study of Protein Tyrosine Phosphatase Receptor Type O Inhibitors. Journal of Chemical Information and Modeling, 2018, 58, 2331-2342.	5.4	8
103	Identification and structureâ€“function analyses of an allosteric inhibitor of the tyrosine phosphatase PTPN22. Journal of Biological Chemistry, 2019, 294, 8653-8663.	3.4	8
104	AlphaSpace 2.0: Representing Concave Biomolecular Surfaces Using Î²-Clusters. Journal of Chemical Information and Modeling, 2020, 60, 1494-1508.	5.4	7
105	Amide Rotation Hindrance Predicts Proteolytic Resistance of Cystine-Knot Peptides. Journal of Physical Chemistry Letters, 2016, 7, 1138-1142.	4.6	6
106	Identification of Secondary Binding Sites on Protein Surfaces for Rational Elaboration of Synthetic Protein Mimics. ACS Chemical Biology, 2021, 16, 1179-1183.	3.4	6
107	De novo Design of SARS-CoV-2 Main Protease Inhibitors. Synlett, 2022, 33, 458-463.	1.8	6
108	Ab Initio QM/MM and Free Energy Calculations of Enzyme Reactions. Lecture Notes in Computational Science and Engineering, 2002, , 333-355.	0.3	6

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109	An in silico mechanistic insight into HDAC8 activation facilitates the discovery of new small-molecule activators. Bioorganic and Medicinal Chemistry, 2020, 28, 115607.	3.0	5
110	Substrateâ€“Enzyme Interactions in Intramembrane Proteolysis: Î³-Secretase as the Prototype. Frontiers in Molecular Neuroscience, 2020, 13, 65.	2.9	3
111	Inhibition of striatal-enriched protein tyrosine phosphatase by targeting computationally revealed cryptic pockets. European Journal of Medicinal Chemistry, 2020, 190, 112131.	5.5	3
112	Substrate interaction inhibits Î³-secretase production of amyloid-Î² peptides. Chemical Communications, 2020, 56, 2578-2581.	4.1	3
113	Introducing sampling entropy in repository based adaptive umbrella sampling. Journal of Chemical Physics, 2009, 131, 214105.	3.0	2
114	Ab Initio Quantum Mechanical/Molecular Mechanical Studies of Histone Modifying Enzymes. Challenges and Advances in Computational Chemistry and Physics, 2009, , 341-350.	0.6	1
115	Functional loop dynamics of the S-component of ECF transporter FolT. Molecular Physics, 2018, 116, 2613-2621.	1.7	0