Darrin M York

List of Publications by Year
in descending order

189 papers	40,640 citations	41344 49 h-index	3487 182 g-index
195 all docs	195 docs citations	195 times ranked	37187 citing authors

#	Article	IF	Citations
1	Inquiry-Based Activities and Games That Engage Students in Learning Atomic Orbitals. Journal of Chemical Education, 2022, 99, 2175-2181.	2.3	6
2	Online Orbital Explorer and BingOrbital Game for Inquiry-Based Activities. Journal of Chemical Education, 2022, 99, 2135-2142.	2.3	5
3	Who stole the proton? Suspect general base guanine found with a smoking gun in the pistol ribozyme. Organic and Biomolecular Chemistry, 2022, , .	2.8	5
4	Combined QM/MM, Machine Learning Path Integral Approach to Compute Free Energy Profiles and Kinetic Isotope Effects in RNA Cleavage Reactions. Journal of Chemical Theory and Computation, 2022, 18, 4304-4317.	5.3	17
5	Introducing a New Bond-Forming Activity in an Archaeal DNA Polymerase by Structure-Guided Enzyme Redesign. ACS Chemical Biology, 2022, 17, 1924-1936.	3.4	3
6	Variational Method for Networkwide Analysis of Relative Ligand Binding Free Energies with Loop Closure and Experimental Constraints. Journal of Chemical Theory and Computation, 2021, 17, 1326-1336.	5.3	16
7	Extension of the Variational Free Energy Profile and Multistate Bennett Acceptance Ratio Methods for High-Dimensional Potential of Mean Force Profile Analysis. Journal of Physical Chemistry A, 2021, 125, 4216-4232.	2.5	15
8	Peripheral Methionine Residues Impact Flavin Photoreduction and Protonation in an Engineered LOV Domain Light Sensor. Biochemistry, 2021, 60, 1148-1164.	2.5	5
9	CHARMM-GUI Free Energy Calculator for Practical Ligand Binding Free Energy Simulations with AMBER. Journal of Chemical Information and Modeling, 2021, 61, 4145-4151.	5.4	24
10	Beneath the Surface: An Investigation of General Chemistry Studentsâ€™ Study Skills to Predict Course Outcomes. Journal of Chemical Education, 2021, 98, 281-292.	2.3	10
11	Development of Range-Corrected Deep Learning Potentials for Fast, Accurate Quantum Mechanical/Molecular Mechanical Simulations of Chemical Reactions in Solution. Journal of Chemical Theory and Computation, 2021, 17, 6993-7009.	5.3	47
12	The L-platform/L-scaffold framework: a blueprint for RNA-cleaving nucleic acid enzyme design. Rna, 2020, 26, 111-125.	3.5	25
13	Improved Alchemical Free Energy Calculations with Optimized Smoothstep Softcore Potentials. Journal of Chemical Theory and Computation, 2020, 16, 5512-5525.	5.3	35
14	Through the Looking CLASS: When Peer Leader Learning Attitudes Are Not What They Seem. Journal of Chemical Education, 2020, 97, 2078-2090.	2.3	4
15	Alchemical Binding Free Energy Calculations in AMBER20: Advances and Best Practices for Drug Discovery. Journal of Chemical Information and Modeling, 2020, 60, 5595-5623.	5.4	177
16	Validation of Free Energy Methods in AMBER. Journal of Chemical Information and Modeling, 2020, 60, 5296-5300.	5.4	19
17	Fast, Accurate, and Reliable Protocols for Routine Calculations of Proteinâ€“Ligand Binding Affinities in Drug Design Projects Using AMBER GPU-TI with ff14SB/GAFF. ACS Omega, 2020, 5, 4611-4619.	3.5	74
18	Confluence of theory and experiment reveals the catalytic mechanism of the Varkud satellite ribozyme. Nature Chemistry, 2020, 12, 193-201.	13.6	33

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19	Molecular simulations of the pistol ribozyme: unifying the interpretation of experimental data and establishing functional links with the hammerhead ribozyme. Rna, 2019, 25, 1439-1456.	3.5	20
20	Predicting Site-Binding Modes of Ions and Water to Nucleic Acids Using Molecular Solvation Theory. Journal of the American Chemical Society, 2019, 141, 2435-2445.	13.7	46
21	Evidence for a Catalytic Strategy to Promote Nucleophile Activation in Metal-Dependent RNA-Cleaving Ribozymes and 8-17 DNAzyme. ACS Catalysis, 2019, 9, 10612-10617.	11.2	22
22	Development of a Robust Indirect Approach for MM â†' QM Free Energy Calculations That Combines Force-Matched Reference Potential and Bennettâ€™s Acceptance Ratio Methods. Journal of Chemical Theory and Computation, 2019, 15, 5543-5562.	5.3	54
23	Dynamical ensemble of the active state and transition state mimic for the RNA-cleaving 8â€"17 DNAzyme in solution. Nucleic Acids Research, 2019, 47, 10282-10295.	14.5	27
24	Using AMBER18 for Relative Free Energy Calculations. Journal of Chemical Information and Modeling, 2019, 59, 3128-3135.	5.4	138
25	Cleaning Up Mechanistic Debris Generated by Twister Ribozymes Using Computational RNA Enzymology. ACS Catalysis, 2019, 9, 5803-5815.	11.2	24
26	An Ontology for Facilitating Discussion of Catalytic Strategies of RNA-Cleaving Enzymes. ACS Chemical Biology, 2019, 14, 1068-1076.	3.4	45
27	Framework for Conducting and Analyzing Crystal Simulations of Nucleic Acids to Aid in Modern Force Field Evaluation. Journal of Physical Chemistry B, 2019, 123, 4611-4624.	2.6	5
28	Quantum Suppression of Intramolecular Deuterium Kinetic Isotope Effects in a Pericyclic Hydrogen Transfer Reaction. Journal of Physical Chemistry A, 2019, 123, 3647-3654.	2.5	1
29	A GPU-Accelerated Parameter Interpolation Thermodynamic Integration Free Energy Method. Journal of Chemical Theory and Computation, 2018, 14, 1564-1582.	5.3	48
30	A Comparison of QM/MM Simulations with and without the Drude Oscillator Model Based on Hydration Free Energies of Simple Solutes. Molecules, 2018, 23, 2695.	3.8	29
31	GPU-Accelerated Molecular Dynamics and Free Energy Methods in Amber18: Performance Enhancements and New Features. Journal of Chemical Information and Modeling, 2018, 58, 2043-2050.	5.4	293
32	On the convergence of multi-scale free energy simulations. Molecular Simulation, 2018, 44, 1062-1081.	2.0	42
33	CATALYTIC STRATEGIES OF NUCLEOLYTIC RIBOZYMES. , 2018, , .		0
34	Toward Fast and Accurate Binding Affinity Prediction with pmemdGTI: An Efficient Implementation of GPU-Accelerated Thermodynamic Integration. Journal of Chemical Theory and Computation, 2017, 13, 3077-3084.	5.3	93
35	Divalent Metal Ion Activation of a Guanine General Base in the Hammerhead Ribozyme: Insights from Molecular Simulations. Biochemistry, 2017, 56, 2985-2994.	2.5	46
36	Quantum mechanical force fields for condensed phase molecular simulations. Journal of Physics Condensed Matter, 2017, 29, 383002.	1.8	22

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37	A Multidimensional B-Spline Correction for Accurate Modeling Sugar Puckering in QM/MM Simulations. Journal of Chemical Theory and Computation, 2017, 13, 3975-3984.	5.3	12
38	Model for the Functional Active State of the TS Ribozyme from Molecular Simulation. Angewandte Chemie - International Edition, 2017, 56, 13392-13395.	13.8	16
39	Model for the Functional Active State of the TS Ribozyme from Molecular Simulation. Angewandte Chemie, 2017, 129, 13577-13580.	2.0	5
40	Kinetic Isotope Effect Analysis of RNA 2â€²- O -Transphosphorylation. Methods in Enzymology, 2017, 596, 433-457.	1.0	3
41	Ambient-Potential Composite Ewald Method for ab Initio Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2016, 12, 2611-2632.	5.3	40
42	The importance of protonation and tautomerization in relative binding affinity prediction: a comparison of AMBER TI and SchrÃ¶dinger FEP. Journal of Computer-Aided Molecular Design, 2016, 30, 533-539.	2.9	25
43	Creation of Academic Social Networks (ASNs) for Effective Online eLearning Communities. ACS Symposium Series, 2016, , 109-126.	0.5	1
44	RepEx: A Flexible Framework for Scalable Replica Exchange Molecular Dynamics Simulations. , 2016, , .		6
45	VR-SCOSMO: A smooth conductor-like screening model with charge-dependent radii for modeling chemical reactions. Journal of Chemical Physics, 2016, 144, 164115.	3.0	3
46	A Two-Metal-Ion-Mediated Conformational Switching Pathway for HDV Ribozyme Activation. ACS Catalysis, 2016, 6, 1853-1869.	11.2	24
47	Ribozyme Catalysis with a Twist: Active State of the Twister Ribozyme in Solution Predicted from Molecular Simulation. Journal of the American Chemical Society, 2016, 138, 3058-3065.	13.7	51
48	Isotope effect analyses provide evidence for an altered transition state for RNA 2â€²-O-transphosphorylation catalyzed by Zn2+. Chemical Communications, 2016, 52, 4462-4465.	4.1	8
49	An active site rearrangement within the Tetrahymena group I ribozyme releases nonproductive interactions and allows formation of catalytic interactions. Rna, 2016, 22, 32-48.	3.5	7
50	Improved ligand geometries in crystallographic refinement usingAFITTinPHENIX. Acta Crystallographica Section D: Structural Biology, 2016, 72, 1062-1072.	2.3	29
51	A Modified Divide-and-Conquer Linear-Scaling Quantum Force Field with Multipolar Charge Densities. , 2016, , 3-31.		3
52	Charge-dependent many-body exchange and dispersion interactions in combined QM/MM simulations. Journal of Chemical Physics, 2015, 143, 234111.	3.0	20
53	Structural fidelity and NMR relaxation analysis in a prototype RNA hairpin. Rna, 2015, 21, 963-974.	3.5	27
54	Assessment of metal-assisted nucleophile activation in the hepatitis delta virus ribozyme from molecular simulation and 3D-RISM. Rna, 2015, 21, 1566-1577.	3.5	18

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55	Competitive interaction of monovalent cations with DNA from 3D-RISM. Nucleic Acids Research, 2015, 43, 8405-8415.	14.5	47
56	Multipolar Ewald Methods, 2: Applications Using a Quantum Mechanical Force Field. Journal of Chemical Theory and Computation, 2015, 11, 451-461.	5.3	19
57	Interpretation of pHâ€“Activity Profiles for Acidâ€“Base Catalysis from Molecular Simulations. Biochemistry, 2015, 54, 1307-1313.	2.5	33
58	Multipolar Ewald Methods, 1: Theory, Accuracy, and Performance. Journal of Chemical Theory and Computation, 2015, 11, 436-450.	5.3	35
59	Characterization of the Three-Dimensional Free Energy Manifold for the Uracil Ribonucleoside from Asynchronous Replica Exchange Simulations. Journal of Chemical Theory and Computation, 2015, 11, 373-377.	5.3	10
60	Comparison of structural, thermodynamic, kinetic and mass transport properties of Mg²⁺ ion models commonly used in biomolecular simulations. Journal of Computational Chemistry, 2015, 36, 970-982.	3.3	79
61	Effect of Zn2+ binding and enzyme active site on the transition state for RNA 2â€²-O-transphosphorylation interpreted through kinetic isotope effects. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2015, 1854, 1795-1800.	2.3	16
62	Heavy atom labeled nucleotides for measurement of kinetic isotope effects. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2015, 1854, 1737-1745.	2.3	10
63	Determination of hepatitis delta virus ribozyme N(â€“1) nucleobase and functional group specificity using internal competition kinetics. Analytical Biochemistry, 2015, 483, 12-20.	2.4	6
64	Multiscale Methods for Computational RNA Enzymology. Methods in Enzymology, 2015, 553, 335-374.	1.0	16
65	Nucleic acid reactivity: Challenges for next-generation semiempirical quantum models. Journal of Computational Chemistry, 2015, 36, 1370-1389.	3.3	14
66	Integration of kinetic isotope effect analyses to elucidate ribonuclease mechanism. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2015, 1854, 1801-1808.	2.3	20
67	Enzyme transition states from theory and experiment. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2015, 1854, 1727-1728.	2.3	5
68	Force Field for Mg²⁺, Mn²⁺, Zn²⁺, and Cd²⁺ Ions That Have Balanced Interactions with Nucleic Acids. Journal of Physical Chemistry B, 2015, 119, 15460-15470.	2.6	95
69	Cationâ€“Anion Interactions within the Nucleic Acid Ion Atmosphere Revealed by Ion Counting. Journal of the American Chemical Society, 2015, 137, 14705-14715.	13.7	65
70	Mechanistic Insights into RNA Transphosphorylation from Kinetic Isotope Effects and Linear Free Energy Relationships of Model Reactions. Chemistry - A European Journal, 2014, 20, 14336-14343.	3.3	29
71	Quantum mechanical study of solvent effects in a prototype SN2 reaction in solution: Clâ¯ attack on CH3Cl. Journal of Chemical Physics, 2014, 140, 054109.	3.0	16
72	Ab initio pathâ€integral calculations of kinetic and equilibrium isotope effects on baseâ€catalyzed RNA transphosphorylation models. Journal of Computational Chemistry, 2014, 35, 1302-1316.	3.3	14

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73	Evidence for the Role of Active Site Residues in the Hairpin Ribozyme from Molecular Simulations along the Reaction Path. Journal of the American Chemical Society, 2014, 136, 7789-7792.	13.7	31
74	Linear free energy relationships in RNA transesterification: theoretical models to aid experimental interpretations. Physical Chemistry Chemical Physics, 2014, 16, 15846-15855.	2.8	18
75	Parametrization of an Orbital-Based Linear-Scaling Quantum Force Field for Noncovalent Interactions. Journal of Chemical Theory and Computation, 2014, 10, 1086-1098.	5.3	29
76	Improvement of DNA and RNA Sugar Pucker Profiles from Semiempirical Quantum Methods. Journal of Chemical Theory and Computation, 2014, 10, 1538-1545.	5.3	50
77	Roadmaps through Free Energy Landscapes Calculated Using the Multidimensional vFEP Approach. Journal of Chemical Theory and Computation, 2014, 10, 24-34.	5.3	58
78	Constant pH Replica Exchange Molecular Dynamics in Explicit Solvent Using Discrete Protonation States: Implementation, Testing, and Validation. Journal of Chemical Theory and Computation, 2014, 10, 1341-1352.	5.3	210
79	Altered (transition) states: mechanisms of solution and enzyme catalyzed RNA 2â€²-O-transphosphorylation. Current Opinion in Chemical Biology, 2014, 21, 96-102.	6.1	34
80	Ion Counting from Explicit-Solvent Simulations and 3D-RISM. Biophysical Journal, 2014, 106, 883-894.	0.5	102
81	Recent Advances toward a General Purpose Linear-Scaling Quantum Force Field. Accounts of Chemical Research, 2014, 47, 2812-2820.	15.6	38
82	Molecular Dynamics Simulation of Nitrobenzene Dioxygenase Using AMBER Force Field. Journal of Chemical Theory and Computation, 2014, 10, 2246-2254.	5.3	27
83	A Variational Linear-Scaling Framework to Build Practical, Efficient Next-Generation Orbital-Based Quantum Force Fields. Journal of Chemical Theory and Computation, 2013, 9, 1417-1427.	5.3	55
84	A New Maximum Likelihood Approach for Free Energy Profile Construction from Molecular Simulations. Journal of Chemical Theory and Computation, 2013, 9, 153-164.	5.3	76
85	Molecular Simulations of RNA 2â€²-O-Transesterification Reaction Models in Solution. Journal of Physical Chemistry B, 2013, 117, 94-103.	2.6	21
86	Bridging the Gap Between Theory and Experiment to Derive a Detailed Understanding of Hammerhead Ribozyme Catalysis. Progress in Molecular Biology and Translational Science, 2013, 120, 25-91.	1.7	8
87	Experimental and computational analysis of the transition state for ribonuclease A-catalyzed RNA 2â€²-O -transphosphorylation. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 13002-13007.	7.1	62
88	A framework for flexible and scalable replica-exchange on production distributed CI. , 2013, , .		3
89	Experimental and computational evidence that ribonuclease A alters the transition state for RNA 2â€²â€Oâ€transphosphorylation. FASEB Journal, 2013, 27, 998.6.	0.5	0
90	Exact Relation between Potential of Mean Force and Free-Energy Profile. Journal of Chemical Theory and Computation, 2012, 8, 3998-4003.	5.3	25

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91	InnenrÃ¼cktitelbild: Characterization of the Reaction Path and Transition States for RNA Transphosphorylation Models from Theory and Experiment (Angew. Chem. 3/2012). Angewandte Chemie, 2012, 124, 847-847.	2.0	0
92	Extended Polarization in Third-Order SCC-DFTB from Chemical-Potential Equalization. Journal of Physical Chemistry A, 2012, 116, 9131-9141.	2.5	42
93	Mapping L1 Ligase Ribozyme Conformational Switch. Journal of Molecular Biology, 2012, 423, 106-122.	4.2	6
94	Density-functional expansion methods: grand challenges. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	30
95	Characterization of the Reaction Path and Transition States for RNA Transphosphorylation Models from Theory and Experiment. Angewandte Chemie - International Edition, 2012, 51, 647-651.	13.8	49
96	Inside Back Cover: Characterization of the Reaction Path and Transition States for RNA Transphosphorylation Models from Theory and Experiment (Angew. Chem. Int. Ed. 3/2012). Angewandte Chemie - International Edition, 2012, 51, 823-823.	13.8	0
97	Characterization of the Structure and Dynamics of the HDV Ribozyme in Different Stages Along the Reaction Path. Journal of Physical Chemistry Letters, 2011, 2, 2538-2543.	4.6	30
98	Active Participation of the Mg²⁺ Ion in the Reaction Coordinate of RNA Self-Cleavage Catalyzed by the Hammerhead Ribozyme. Journal of Chemical Theory and Computation, 2011, 7, 1-3.	5.3	50
99	Density-functional expansion methods: Generalization of the auxiliary basis. Journal of Chemical Physics, 2011, 134, 194103.	3.0	11
100	Influence of C-5 substituted cytosine and related nucleoside analogs on the formation of benzo[a]pyrene diol epoxide-dG adducts at CG base pairs of DNA. Nucleic Acids Research, 2011, 39, 3988-4006.	14.5	40
101	Insights into the Role of Conformational Transitions and Metal Ion Binding in RNA Catalysis from Molecular Simulations. Annual Reports in Computational Chemistry, 2010, 6, 168-200.	1.7	1
102	Density-functional expansion methods: Evaluation of LDA, GGA, and meta-GGA functionals and different integral approximations. Journal of Chemical Physics, 2010, 133, 244107.	3.0	37
103	Identification of dynamical hinge points of the L1 ligase molecular switch. Rna, 2010, 16, 769-780.	3.5	7
104	Exocyclic Deoxyadenosine Adducts of 1,2,3,4-Diepoxybutane: Synthesis, Structural Elucidation, and Mechanistic Studies. Chemical Research in Toxicology, 2010, 23, 118-133.	3.3	34
105	Computational Mutagenesis Studies of Hammerhead Ribozyme Catalysis. Journal of the American Chemical Society, 2010, 132, 13505-13518.	13.7	19
106	Molecular Dynamics Simulation of Bovine Pancreatic Ribonuclease Aâˆ’CpA and Transition State-like Complexes. Journal of Physical Chemistry B, 2010, 114, 7371-7382.	2.6	25
107	Accurate Proton Affinity and Gas-Phase Basicity Values for Molecules Important in Biocatalysis. Journal of Physical Chemistry B, 2010, 114, 13911-13921.	2.6	127
108	CHARMM: The biomolecular simulation program. Journal of Computational Chemistry, 2009, 30, 1545-1614.	3.3	7,077

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109	Density functional study of the influence of C5 cytosine substitution in base pairs with guanine. Theoretical Chemistry Accounts, 2009, 122, 179-188.	1.4	18
110	Threshold Occupancy and Specific Cation Binding Modes in the Hammerhead Ribozyme Active Site are Required for Active Conformation. Journal of Molecular Biology, 2009, 388, 195-206.	4.2	43
111	Unraveling the Mechanisms of Ribozyme Catalysis with Multiscale Simulations. Challenges and Advances in Computational Chemistry and Physics, 2009, , 377-408.	0.6	1
112	Extension of adaptive tree code and fast multipole methods to high angular momentum particle charge densities. Journal of Computational Chemistry, 2008, 29, 1895-1904.	3.3	17
113	Solvent Structure and Hammerhead RibozymeÂCatalysis. Chemistry and Biology, 2008, 15, 332-342.	6.0	104
114	Spherical tensor gradient operator method for integral rotation: A simple, efficient, and extendable alternative to Slaterâ€"Koster tables. Journal of Chemical Physics, 2008, 129, 016102.	3.0	6
115	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
116	Role of Mg²⁺ in Hammerhead Ribozyme Catalysis from Molecular Simulation. Journal of the American Chemical Society, 2008, 130, 3053-3064.	13.7	102
117	Quantum Mechanical/Molecular Mechanical Simulation Study of the Mechanism of Hairpin Ribozyme Catalysis. Journal of the American Chemical Society, 2008, 130, 4680-4691.	13.7	79
118	Origin of Mutational Effects at the C3 and G8 Positions on Hammerhead Ribozyme Catalysis from Molecular Dynamics Simulations. Journal of the American Chemical Society, 2008, 130, 7168-7169.	13.7	19
119	Contracted auxiliary Gaussian basis integral and derivative evaluation. Journal of Chemical Physics, 2008, 128, 064104.	3.0	23
120	Electrostatic interactions in the hairpin ribozyme account for the majority of the rate acceleration without chemical participation by nucleobases. Rna, 2008, 14, 1501-1507.	3.5	47
121	Charge-dependent model for many-body polarization, exchange, and dispersion interactions in hybrid quantum mechanicalâˆ•molecular mechanical calculations. Journal of Chemical Physics, 2007, 127, 194101.	3.0	56
122	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
123	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
124	Insight into the Role of Mg2+ in Hammerhead Ribozyme Catalysis from X-ray Crystallography and Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2007, 3, 325-327.	5.3	38
125	CHARMM force field parameters for simulation of reactive intermediates in native and thio-substituted ribozymes. Journal of Computational Chemistry, 2007, 28, 495-507.	3.3	49
126	Enzyme Dynamics and Tunneling Enhanced by Compression in the Hydrogen Abstraction Catalyzed by Soybean Lipoxygenase-1. Journal of Physical Chemistry B, 2006, 110, 24708-24719.	2.6	51

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127	Nucleophilic Attack on Phosphate Diesters:Â A Density Functional Study of Inâ^'Line Reactivity in Dianionic, Monoanionic, and Neutral Systems. Journal of Physical Chemistry B, 2006, 110, 11525-11539.	2.6	71
128	Normal Modes of Redox-Active Tyrosine:Â Conformation Dependence and Comparison to Experiment. Journal of Physical Chemistry B, 2006, 110, 10970-10981.	2.6	31
129	Multilevel and Density Functional Electronic Structure Calculations of Proton Affinities and Gas-Phase Basicities Involved in Biological Phosphoryl Transferâ€. Journal of Physical Chemistry A, 2006, 110, 791-797.	2.5	17
130	QCRNA 1.0: A database of quantum calculations for RNA catalysis. Journal of Molecular Graphics and Modelling, 2006, 25, 423-433.	2.4	26
131	Transesterification Thio Effects of Phosphate Diesters:Â Free Energy Barriers and Kinetic and Equilibrium Isotope Effects from Density-Functional Theoryâ€. Biochemistry, 2006, 45, 10043-10053.	2.5	67
132	A charge-scaling implementation of the variational electrostatic projection method. Journal of Computational Chemistry, 2006, 27, 103-115.	3.3	10
133	Theoretical methods that help understanding the structure and reactivity of gas phase ions. International Journal of Mass Spectrometry, 2005, 240, 37-99.	1.5	104
134	Pseudorotation Barriers of Biological Oxyphosphoranes: A Challenge for Simulations of Ribozyme Catalysis. Chemistry - A European Journal, 2005, 11, 2081-2093.	3.3	54
135	Ellipticity: A Convenient Tool To Characterize Electrocyclic Reactions. Chemistry - A European Journal, 2005, 11, 1734-1738.	3.3	71
136	High-order discretization schemes for biochemical applications of boundary element solvation and variational electrostatic projection methods. Journal of Chemical Physics, 2005, 122, 194110.	3.0	14
137	Improvement of semiempirical response properties with charge-dependent response density. Journal of Chemical Physics, 2005, 123, 164108.	3.0	53
138	The contribution of phosphate-phosphate repulsions to the free energy of DNA bending. Nucleic Acids Research, 2005, 33, 1257-1268.	14.5	35
139	Kinetic isotope effects on thio-substituted biological phosphoryl transfer reactions from density-functional theory. Chemical Communications, 2005, , 3909.	4.1	17
140	An Efficient Linear-Scaling Ewald Method for Long-Range Electrostatic Interactions in Combined QM/MM Calculations. Journal of Chemical Theory and Computation, 2005, 1, 2-13.	5.3	258
141	Smooth Solvation Method for d-Orbital Semiempirical Calculations of Biological Reactions. 1. Implementation. Journal of Physical Chemistry B, 2005, 109, 9799-9809.	2.6	30
142	Density Functional Study of the In-Line Mechanism of Methanolysis of Cyclic Phosphate and Thiophosphate Esters in Solution:Â Insight into Thio Effects in RNA Transesterification. Journal of Physical Chemistry B, 2005, 109, 19987-20003.	2.6	34
143	A Semiempirical Quantum Model for Hydrogen-Bonded Nucleic Acid Base Pairs. Journal of Chemical Theory and Computation, 2005, 1, 1275-1285.	5.3	45
144	Variational Electrostatic Projection (VEP) Methods for Efficient Modeling of the Macromolecular Electrostatic and Solvation Environment in Activated Dynamics Simulations. Journal of Physical Chemistry B, 2005, 109, 536-556.	2.6	26

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145	Benchmark calculations of proton affinities and gas-phase basicities of molecules important in the study of biological phosphoryl transfer. Physical Chemistry Chemical Physics, 2005, 7, 3070.	2.8	76
146	Smooth Solvation Method for d-Orbital Semiempirical Calculations of Biological Reactions. 2. Application to Transphosphorylation Thio Effects in Solution. Journal of Physical Chemistry B, 2005, 109, 9810-9817.	2.6	18
147	Theoretical Studies of Dissociative Phosphoryl Transfer in Interconversion of Phosphoenolpyruvate to Phosphonopyruvate:Â Solvent Effects, Thio Effects, and Implications for Enzymatic Reactions. Journal of Physical Chemistry B, 2005, 109, 13827-13834.	2.6	20
148	Solvent Polarization and Kinetic Isotope Effects in Nitroethane Deprotonation and Implications to the Nitroalkane Oxidase Reaction. Journal of the American Chemical Society, 2005, 127, 16374-16375.	13.7	50
149	Design and application of a multicoefficient correlation method for dispersion interactions. Journal of Chemical Physics, 2004, 120, 590-602.	3.0	8
150	Many-body force field models based solely on pairwise Coulomb screening do not simultaneously reproduce correct gas-phase and condensed-phase polarizability limits. Journal of Chemical Physics, 2004, 120, 9903-9906.	3.0	63
151	Complete basis set extrapolated potential energy, dipole, and polarizability surfaces of alkali halide ion-neutral weakly avoided crossings with and without applied electric fields. Journal of Chemical Physics, 2004, 120, 7939-7948.	3.0	34
152	Structure and binding of Mg(II) ions and di-metal bridge complexes with biological phosphates and phosphoranes. Journal of Biological Inorganic Chemistry, 2004, 9, 807-817.	2.6	27
153	Quantum descriptors for biological macromolecules from linear-scaling electronic structure methods. Proteins: Structure, Function and Bioinformatics, 2004, 56, 724-737.	2.6	50
154	High-level ab initio methods for calculation of potential energy surfaces of van der Waals complexes. International Journal of Quantum Chemistry, 2004, 98, 388-408.	2.0	35
155	Pseudorotation of Natural and Chemically Modified Biological Phosphoranes: Implications for RNA Catalysis. ChemPhysChem, 2004, 5, 1045-1049.	2.1	32
156	Pseudorotation of Natural and Chemically Modified Biological Phosphoranes: Implications for RNA Catalysis. ChemPhysChem, 2004, 5, 1266-1266.	2.1	1
157	The Structure and Stability of Biological Metaphosphate, Phosphate, and Phosphorane Compounds in the Gas Phase and in Solution. Journal of the American Chemical Society, 2004, 126, 1654-1665.	13.7	94
158	Hybrid QM/MM Study of Thio Effects in Transphosphorylation Reactions:Â The Role of Solvation. Journal of the American Chemical Society, 2004, 126, 7504-7513.	13.7	56
159	Theoretical Study of the Vinyl Allene Oxide to Cyclopent-2-en-1-one Rearrangement:â€‰ Mechanism, Torquoselectivity and Solvent Effects. Journal of Organic Chemistry, 2004, 69, 3635-3644.	3.2	35
160	Parameterization of semiempirical methods to treat nucleophilic attacks to biological phosphates: AM1/d parameters for phosphorus. Theoretical Chemistry Accounts, 2003, 109, 149-159.	1.4	40
161	Fast approximate methods for calculating nucleic acid base pair interaction energies. Journal of Computational Chemistry, 2003, 24, 57-67.	3.3	30
162	Insights into the Regioselectivity and RNA-binding Affinity of HIV-1 Nucleocapsid Protein from Linear-scaling Quantum Methods. Journal of Molecular Biology, 2003, 330, 993-1004.	4.2	38

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