Darrin M York

List of Publications by Citations

186 papers	31,975 citations	47 h-index	178 g-index
195 ext. papers	36,840 ext. citations	6 avg, IF	7.02 L-index

#	Paper	IF	Citations
186	Particle mesh Ewald: An N?log(N) method for Ewald sums in large systems. *Journal of Chemical Physics*, **1993**, 98, 10089-10092	3.9	19280
185	CHARMM: the biomolecular simulation program. *Journal of Computational Chemistry*, **2009**, 30, 1545-614	3.5	5515
184	The effect of long-range electrostatic interactions in simulations of macromolecular crystals: A comparison of the Ewald and truncated list methods. *Journal of Chemical Physics*, **1993**, 99, 8345-8348	3.9	498
183	A Smooth Solvation Potential Based on the Conductor-Like Screening Model. *Journal of Physical Chemistry A*, **1999**, 103, 11060-11079	2.8	306
182	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
181	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	6.4	217
180	A chemical potential equalization method for molecular simulations. *Journal of Chemical Physics*, **1996**, 104, 159-172	3.9	201
179	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	6.1	165
178	Atomic-level accuracy in simulations of large protein crystals. *Proceedings of the National Academy of Sciences of the United States of America*, **1994**, 91, 8715-8	11.5	164
177	Toward the Accurate Modeling of DNA: The Importance of Long-Range Electrostatics. *Journal of the American Chemical Society*, **1995**, 117, 5001-5002	16.4	162
176	Linear-scaling semiempirical quantum calculations for macromolecules. *Journal of Chemical Physics*, **1996**, 105, 2744-2750	3.9	155
175	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	6.4	149
174	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
173	Accurate proton affinity and gas-phase basicity values for molecules important in biocatalysis. *Journal of Physical Chemistry B*, **2010**, 114, 13911-21	3.4	105
172	The fast Fourier Poisson method for calculating Ewald sums. *Journal of Chemical Physics*, **1994**, 101, 3298-3300	3.9	98
171	Theoretical methods that help understanding the structure and reactivity of gas phase ions. *International Journal of Mass Spectrometry*, **2005**, 240, 37-99	1.9	95
170	Role of Mg2+ in hammerhead ribozyme catalysis from molecular simulation. *Journal of the American Chemical Society*, **2008**, 130, 3053-64	16.4	93

169	Solvent structure and hammerhead ribozyme catalysis. *Chemistry and Biology*, **2008**, 15, 332-42		92
168	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, 1654-65	16.4	92
167	Ion counting from explicit-solvent simulations and 3D-RISM. *Biophysical Journal*, **2014**, 106, 883-94	2.9	77
166	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
165	Quantum mechanical/molecular mechanical simulation study of the mechanism of hairpin ribozyme catalysis. *Journal of the American Chemical Society*, **2008**, 130, 4680-91	16.4	74
164	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, 3070-9	3.6	72
163	Hybrid QM/MM study of thio effects in transphosphorylation reactions. *Journal of the American Chemical Society*, **2003**, 125, 7178-9	16.4	69
162	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	6.4	66
161	Force Field for Mg(2+), Mn(2+), Zn(2+), and Cd(2+) Ions That Have Balanced Interactions with Nucleic Acids. *Journal of Physical Chemistry B*, **2015**, 119, 15460-70	3.4	66
160	Nucleophilic attack on phosphate diesters: a density functional study of in-line reactivity in dianionic, monoanionic, and neutral systems. *Journal of Physical Chemistry B*, **2006**, 110, 11525-39	3.4	66
159	Transesterification thio effects of phosphate diesters: free energy barriers and kinetic and equilibrium isotope effects from density-functional theory. *Biochemistry*, **2006**, 45, 10043-53	3.2	64
158	Ellipticity: a convenient tool to characterize electrocyclic reactions. *Chemistry - A European Journal*, **2005**, 11, 1734-8	4.8	64
157	Quantum Mechanical Treatment of Biological Macromolecules in Solution Using Linear-Scaling Electronic Structure Methods. *Physical Review Letters*, **1998**, 80, 5011-5014	7.4	63
156	Using AMBER18 for Relative Free Energy Calculations. *Journal of Chemical Information and Modeling*, **2019**, 59, 3128-3135	6.1	62
155	A New Maximum Likelihood Approach for Free Energy Profile Construction from Molecular Simulations. *Journal of Chemical Theory and Computation*, **2013**, 9, 153-164	6.4	59
154	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, 9903-6	3.9	59
153	Alchemical Binding Free Energy Calculations in AMBER20: Advances and Best Practices for Drug Discovery. *Journal of Chemical Information and Modeling*, **2020**, 60, 5595-5623	6.1	56
152	Hybrid QM/MM study of thio effects in transphosphorylation reactions: the role of solvation. *Journal of the American Chemical Society*, **2004**, 126, 7504-13	16.4	54

151	Quantum Mechanical Study of Aqueous Polarization Effects on Biological Macromolecules. *Journal of the American Chemical Society*, **1996**, 118, 10940-10941	16.4	54
150	Charge-dependent model for many-body polarization, exchange, and dispersion interactions in hybrid quantum mechanical/molecular mechanical calculations. *Journal of Chemical Physics*, **2007**, 127, 194101	3.9	53
149	Comparison of structural, thermodynamic, kinetic and mass transport properties of Mg(2+) ion models commonly used in biomolecular simulations. *Journal of Computational Chemistry*, **2015**, 36, 970-82	3.5	52
148	Experimental and computational analysis of the transition state for ribonuclease A-catalyzed RNA 2SO-transphosphorylation. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 13002-7	11.5	52
147	Pseudorotation barriers of biological oxyphosphoranes: a challenge for simulations of ribozyme catalysis. *Chemistry - A European Journal*, **2005**, 11, 2081-93	4.8	51
146	Solvent polarization and kinetic isotope effects in nitroethane deprotonation and implications to the nitroalkane oxidase reaction. *Journal of the American Chemical Society*, **2005**, 127, 16374-5	16.4	50
145	Density-functional calculations of the structure and stability of C240. *Physical Review B*, **1994**, 49, 8526-8528	3.7	50
144	Enzyme dynamics and tunneling enhanced by compression in the hydrogen abstraction catalyzed by soybean lipoxygenase-1. *Journal of Physical Chemistry B*, **2006**, 110, 24708-19	3.4	49
143	Improvement of semiempirical response properties with charge-dependent response density. *Journal of Chemical Physics*, **2005**, 123, 164108	3.9	49
142	Cation-Anion Interactions within the Nucleic Acid Ion Atmosphere Revealed by Ion Counting. *Journal of the American Chemical Society*, **2015**, 137, 14705-15	16.4	48
141	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	6.4	48
140	Active participation of Mg ion in the reaction coordinate of RNA self-cleavage catalyzed by the hammerhead ribozyme. *Journal of Chemical Theory and Computation*, **2011**, 7, 1-3	6.4	47
139	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, 3058-65	16.4	46
138	Quantum descriptors for biological macromolecules from linear-scaling electronic structure methods. *Proteins: Structure, Function and Bioinformatics*, **2004**, 56, 724-37	4.2	46
137	Spectroscopic properties of tyrosyl radicals in dipeptides. *Journal of the American Chemical Society*, **2002**, 124, 5496-505	16.4	46
136	Roadmaps through free energy landscapes calculated using the multi-dimensional vFEP approach. *Journal of Chemical Theory and Computation*, **2014**, 10, 24-34	6.4	45
135	Parameterization and efficient implementation of a solvent model for linear-scaling semiempirical quantum mechanical calculations of biological macromolecules. *Chemical Physics Letters*, **1996**, 263, 297-304	2.5	45
134	Electrostatic interactions in the hairpin ribozyme account for the majority of the rate acceleration without chemical participation by nucleobases. *Rna*, **2008**, 14, 1501-7	5.8	44

133	Characterization of the reaction path and transition states for RNA transphosphorylation models from theory and experiment. *Angewandte Chemie - International Edition*, **2012**, 51, 647-51	16.4	43
132	A Semiempirical Quantum Model for Hydrogen-Bonded Nucleic Acid Base Pairs. *Journal of Chemical Theory and Computation*, **2005**, 1, 1275-85	6.4	42
131	Theoretical studies on the hydrolysis of phosphate diesters in the gas phase, solution, and RNase A. *International Journal of Quantum Chemistry*, **2002**, 86, 10-26	2.1	40
130	Improvement of DNA and RNA Sugar Pucker Profiles from Semiempirical Quantum Methods. *Journal of Chemical Theory and Computation*, **2014**, 10, 1538-1545	6.4	38
129	Extended polarization in third-order SCC-DFTB from chemical-potential equalization. *Journal of Physical Chemistry A*, **2012**, 116, 9131-41	2.8	38
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127	CHARMM force field parameters for simulation of reactive intermediates in native and thio-substituted ribozymes. *Journal of Computational Chemistry*, **2007**, 28, 495-507	3.5	38
126	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	20.1	37
125	Insight into the role of Mg in hammerhead ribozyme catalysis from X-ray crystallography and molecular dynamics simulation. *Journal of Chemical Theory and Computation*, **2007**, 3, 325-327	6.4	37
124	Parameterization of semiempirical methods to treat nucleophilic attacks to biological phosphates: AM1/d parameters for phosphorus. *Theoretical Chemistry Accounts*, **2003**, 109, 149-159	1.9	37
123	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	6.5	36
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120	Recent advances toward a general purpose linear-scaling quantum force field. *Accounts of Chemical Research*, **2014**, 47, 2812-20	24.3	34
119	Exocyclic deoxyadenosine adducts of 1,2,3,4-diepoxybutane: synthesis, structural elucidation, and mechanistic studies. *Chemical Research in Toxicology*, **2010**, 23, 118-33	4	34
118	Density functional study of the in-line mechanism of methanolysis of cyclic phosphate and thiophosphate esters in solution: insight into thio effects in RNA transesterification. *Journal of Physical Chemistry B*, **2005**, 109, 19987-20003	3.4	33
117	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	2.1	33
116	Competitive interaction of monovalent cations with DNA from 3D-RISM. *Nucleic Acids Research*, **2015**, 43, 8405-15	20.1	32

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114	Fast, Accurate, and Reliable Protocols for Routine Calculations of Protein-Ligand Binding Affinities in Drug Design Projects Using AMBER GPU-TI with ff14SB/GAFF. *ACS Omega*, **2020**, 5, 4611-4619	3.9	31
113	Normal modes of redox-active tyrosine: conformation dependence and comparison to experiment. *Journal of Physical Chemistry B*, **2006**, 110, 10970-81	3.4	31
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111	Multipolar Ewald methods, 1: theory, accuracy, and performance. *Journal of Chemical Theory and Computation*, **2015**, 11, 436-50	6.4	30
110	Characterization of the Structure and Dynamics of the HDV Ribozyme at Different Stages Along the Reaction Path. *Journal of Physical Chemistry Letters*, **2011**, 2, 2538-2543	6.4	30
109	The contribution of phosphate-phosphate repulsions to the free energy of DNA bending. *Nucleic Acids Research*, **2005**, 33, 1257-68	20.1	30
108	Smooth solvation method for d-orbital semiempirical calculations of biological reactions. 1. Implementation. *Journal of Physical Chemistry B*, **2005**, 109, 9799-809	3.4	30
107	Fast approximate methods for calculating nucleic acid base pair interaction energies. *Journal of Computational Chemistry*, **2003**, 24, 57-67	3.5	30
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103	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	16.4	27
102	Parametrization of an Orbital-Based Linear-Scaling Quantum Force Field for Noncovalent Interactions. *Journal of Chemical Theory and Computation*, **2014**, 10, 1086-1098	6.4	27
101	Interpretation of pH-activity profiles for acid-base catalysis from molecular simulations. *Biochemistry*, **2015**, 54, 1307-13	3.2	27
100	Density-functional expansion methods: Grand challenges. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	27
99	Density-functional expansion methods: evaluation of LDA, GGA, and meta-GGA functionals and different integral approximations. *Journal of Chemical Physics*, **2010**, 133, 244107	3.9	27
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93	Ambient-Potential Composite Ewald Method for ab Initio Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation. *Journal of Chemical Theory and Computation*, **2016**, 12, 2611-32	6.4	26
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85	Exact Relation between Potential of Mean Force and Free-Energy Profile. *Journal of Chemical Theory and Computation*, **2012**, 8, 3998-4003	6.4	21
84	Molecular simulations of RNA 2SO-transesterification reaction models in solution. *Journal of Physical Chemistry B*, **2013**, 117, 94-103	3.4	21
83	Molecular Dynamics Simulation of Nitrobenzene Dioxygenase Using AMBER Force Field. *Journal of Chemical Theory and Computation*, **2014**, 10, 2246-2254	6.4	20
82	Molecular dynamics simulation of bovine pancreatic ribonuclease A-CpA and transition state-like complexes. *Journal of Physical Chemistry B*, **2010**, 114, 7371-82	3.4	20
81	Contracted auxiliary Gaussian basis integral and derivative evaluation. *Journal of Chemical Physics*, **2008**, 128, 064104	3.9	19
80	Quantum Mechanical Characterization of Nucleic Acids in Solution:A Linear-Scaling Study of Charge Fluctuations in DNA and RNA. *Journal of Physical Chemistry B*, **2002**, 106, 7693-7703	3.4	19

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73	Multipolar Ewald methods, 2: applications using a quantum mechanical force field. *Journal of Chemical Theory and Computation*, **2015**, 11, 451-61	6.4	17
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70	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, 7168-9	16.4	17
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68	Multilevel and density functional electronic structure calculations of proton affinities and gas-phase basicities involved in biological phosphoryl transfer. *Journal of Physical Chemistry A*, **2006**, 110, 791-7	2.8	17
67	Improved Alchemical Free Energy Calculations with Optimized Smoothstep Softcore Potentials. *Journal of Chemical Theory and Computation*, **2020**, 16, 5512-5525	6.4	17
66	Model for the Functional Active State of the TS Ribozyme from Molecular Simulation. *Angewandte Chemie - International Edition*, **2017**, 56, 13392-13395	16.4	16
65	Assessment of metal-assisted nucleophile activation in the hepatitis delta virus ribozyme from molecular simulation and 3D-RISM. *Rna*, **2015**, 21, 1566-77	5.8	16
64	Density-Functional Study of the Geometries, Stabilities, and Bond Energies of Group IIIV (13□15) Four-Membered-Ring Compounds. *Journal of the American Chemical Society*, **1996**, 118, 5732-5736	16.4	16
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62	Cleaning Up Mechanistic Debris Generated by Twister Ribozymes Using Computational RNA Enzymology. *ACS Catalysis*, **2019**, 9, 5803-5815	13.1	15

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54	Linear free energy relationships in RNA transesterification: theoretical models to aid experimental interpretations. *Physical Chemistry Chemical Physics*, **2014**, 16, 15846-55	3.6	14
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51	Nucleic acid reactivity: challenges for next-generation semiempirical quantum models. *Journal of Computational Chemistry*, **2015**, 36, 1370-89	3.5	13
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37	Validation of Free Energy Methods in AMBER. *Journal of Chemical Information and Modeling*, **2020**, 60, 5296-5300	6.1	7
36	Design and application of a multicoefficient correlation method for dispersion interactions. *Journal of Chemical Physics*, **2004**, 120, 590-602	3.9	7
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30	An active site rearrangement within the Tetrahymena group I ribozyme releases nonproductive interactions and allows formation of catalytic interactions. *Rna*, **2016**, 22, 32-48	5.8	5
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