Adrian E Roitberg

List of Publications by Citations

101 papers	12,892 citations	43 h-index	113 g-index
113 ext. papers	15,425 ext. citations	6.7 avg, IF	6.64 L-index

#	Paper	IF	Citations
101	Comparison of multiple Amber force fields and development of improved protein backbone parameters. *Proteins: Structure, Function and Bioinformatics*, **2006**, 65, 712-25	4.2	5087
100	MMPBSA.py: An Efficient Program for End-State Free Energy Calculations. *Journal of Chemical Theory and Computation*, **2012**, 8, 3314-21	6.4	1807
99	ANI-1: an extensible neural network potential with DFT accuracy at force field computational cost. *Chemical Science*, **2017**, 8, 3192-3203	9.4	705
98	Long-Time-Step Molecular Dynamics through Hydrogen Mass Repartitioning. *Journal of Chemical Theory and Computation*, **2015**, 11, 1864-74	6.4	453
97	Less is more: Sampling chemical space with active learning. *Journal of Chemical Physics*, **2018**, 148, 241733	3.9	249
96	Mo/llerPlesset perturbation theory applied to vibrational problems. *Journal of Chemical Physics*, **1996**, 105, 11261-11267	3.9	214
95	Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning. *Nature Communications*, **2019**, 10, 2903	17.4	213
94	QSAR without borders. *Chemical Society Reviews*, **2020**, 49, 3525-3564	58.5	196
93	Implementation of the SCC-DFTB method for hybrid QM/MM simulations within the amber molecular dynamics package. *Journal of Physical Chemistry A*, **2007**, 111, 5655-64	2.8	183
92	Nonadiabatic excited-state molecular dynamics: modeling photophysics in organic conjugated materials. *Accounts of Chemical Research*, **2014**, 47, 1155-64	24.3	174
91	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
90	Nonadiabatic excited-state molecular dynamics modeling of photoinduced dynamics in conjugated molecules. *Journal of Physical Chemistry B*, **2011**, 115, 5402-14	3.4	155
89	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
88	Identification of unavoided crossings in nonadiabatic photoexcited dynamics involving multiple electronic states in polyatomic conjugated molecules. *Journal of Chemical Physics*, **2012**, 137, 014512	3.9	140
87	The catalytic mechanism of peptidylglycine alpha-hydroxylating monooxygenase investigated by computer simulation. *Journal of the American Chemical Society*, **2006**, 128, 12817-28	16.4	126
86	Bad Seeds Sprout Perilous Dynamics: Stochastic Thermostat Induced Trajectory Synchronization in Biomolecules. *Journal of Chemical Theory and Computation*, **2009**, 5, 1624-31	6.4	123
85	ANI-1, A data set of 20 million calculated off-equilibrium conformations for organic molecules. *Scientific Data*, **2017**, 4, 170193	8.2	114

84	Non-adiabatic Excited-State Molecular Dynamics: Theory and Applications for Modeling Photophysics in Extended Molecular Materials. *Chemical Reviews*, **2020**, 120, 2215-2287	68.1	113
83	A DFT-Based QM-MM Approach Designed for the Treatment of Large Molecular Systems: Application to Chorismate Mutase. *Journal of Physical Chemistry B*, **2003**, 107, 13728-13736	3.4	110
82	Exchange frequency in replica exchange molecular dynamics. *Journal of Chemical Physics*, **2008**, 128, 024103	3.9	106
81	Nonadiabatic excited-state molecular dynamics: treatment of electronic decoherence. *Journal of Chemical Physics*, **2013**, 138, 224111	3.9	101
80	Multidimensional Replica Exchange Molecular Dynamics Yields a Converged Ensemble of an RNA Tetranucleotide. *Journal of Chemical Theory and Computation*, **2014**, 10, 492-499	6.4	99
79	pH-Dependent conformational changes in proteins and their effect on experimental pK(a)s: the case of Nitrophorin 4. *PLoS Computational Biology*, **2012**, 8, e1002761	5	90
78	Exchange Often and Properly in Replica Exchange Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2010**, 6, 2804-8	6.4	89
77	Nonadiabatic excited-state molecular dynamics: numerical tests of convergence and parameters. *Journal of Chemical Physics*, **2012**, 136, 054108	3.9	80
76	Constant pH replica exchange molecular dynamics in biomolecules using a discrete protonation model. *Journal of Chemical Theory and Computation*, **2010**, 6, 1401-1412	6.4	79
75	Enhancing Conformation and Protonation State Sampling of Hen Egg White Lysozyme Using pH Replica Exchange Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2012**, 8, 4393-404	6.4	71
74	Nonadiabatic molecular dynamics simulations of the energy transfer between building blocks in a phenylene ethynylene dendrimer. *Journal of Physical Chemistry A*, **2009**, 113, 7535-42	2.8	71
73	Coupling of replica exchange simulations to a non-Boltzmann structure reservoir. *Journal of Physical Chemistry B*, **2007**, 111, 2415-8	3.4	71
72	Transferable Dynamic Molecular Charge Assignment Using Deep Neural Networks. *Journal of Chemical Theory and Computation*, **2018**, 14, 4687-4698	6.4	65
71	Discovering a Transferable Charge Assignment Model Using Machine Learning. *Journal of Physical Chemistry Letters*, **2018**, 9, 4495-4501	6.4	65
70	Free Energy Calculations with Non-Equilibrium Methods: Applications of the Jarzynski Relationship. *Theoretical Chemistry Accounts*, **2006**, 116, 338-346	1.9	65
69	Computing Alchemical Free Energy Differences with Hamiltonian Replica Exchange Molecular Dynamics (H-REMD) Simulations. *Journal of Chemical Theory and Computation*, **2011**, 7, 2721-2727	6.4	59
68	Unidirectional Energy Transfer in Conjugated Molecules: The Crucial Role of High-Frequency C?C Bonds. *Journal of Physical Chemistry Letters*, **2010**, 1, 2699-2704	6.4	53
67	Energy transfer in the nanostar: the role of coulombic coupling and dynamics. *Journal of Physical Chemistry B*, **2005**, 109, 11512-9	3.4	50

66	TorchANI: A Free and Open Source PyTorch-Based Deep Learning Implementation of the ANI Neural Network Potentials. *Journal of Chemical Information and Modeling*, **2020**, 60, 3408-3415	6.1	49
65	Shishiodoshi unidirectional energy transfer mechanism in phenylene ethynylene dendrimers. *Journal of Chemical Physics*, **2012**, 137, 22A526	3.9	49
64	Coherent exciton-vibrational dynamics and energy transfer in conjugated organics. *Nature Communications*, **2018**, 9, 2316	17.4	48
63	The ANI-1ccx and ANI-1x data sets, coupled-cluster and density functional theory properties for molecules. *Scientific Data*, **2020**, 7, 134	8.2	47
62	Artifacts due to trivial unavoided crossings in the modeling of photoinduced energy transfer dynamics in extended conjugated molecules. *Chemical Physics Letters*, **2013**, 590, 208-213	2.5	47
61	Electronic Delocalization, Vibrational Dynamics, and Energy Transfer in Organic Chromophores. *Journal of Physical Chemistry Letters*, **2017**, 8, 3020-3031	6.4	45
60	Extending the Applicability of the ANI Deep Learning Molecular Potential to Sulfur and Halogens. *Journal of Chemical Theory and Computation*, **2020**, 16, 4192-4202	6.4	45
59	Analysis of state-specific vibrations coupled to the unidirectional energy transfer in conjugated dendrimers. *Journal of Physical Chemistry A*, **2012**, 116, 9802-10	2.8	40
58	Solvent-induced symmetry breaking of nitrate ion in aqueous clusters: A quantum-classical simulation study. *Journal of Chemical Physics*, **2002**, 117, 2718-2725	3.9	40
57	Dynamics of Energy Transfer in a Conjugated Dendrimer Driven by Ultrafast Localization of Excitations. *Journal of the American Chemical Society*, **2015**, 137, 11637-44	16.4	39
56	pH-replica exchange molecular dynamics in proteins using a discrete protonation method. *Journal of Physical Chemistry B*, **2012**, 116, 8805-11	3.4	37
55	Structure-Activity Relationships of Benzenesulfonamide-Based Inhibitors towards Carbonic Anhydrase Isoform Specificity. *ChemBioChem*, **2017**, 18, 213-222	3.8	35
54	Experimental and Theoretical Investigation of Sodiated Multimers of Steroid Epimers with Ion Mobility-Mass Spectrometry. *Journal of the American Society for Mass Spectrometry*, **2017**, 28, 323-331	3.5	32
53	pH-REMD simulations indicate that the catalytic aspartates of HIV-1 protease exist primarily in a monoprotonated state. *Journal of Physical Chemistry B*, **2014**, 118, 12577-85	3.4	32
52	Photoexcited Nonadiabatic Dynamics of Solvated Push-Pull π-Conjugated Oligomers with the NEXMD Software. *Journal of Chemical Theory and Computation*, **2018**, 14, 3955-3966	6.4	30
51	Electronic Spectra of the Nanostar Dendrimer: Theory and Experiment. *Journal of Physical Chemistry C*, **2010**, 114, 20702-20712	3.8	30
50	Optimization of Umbrella Sampling Replica Exchange Molecular Dynamics by Replica Positioning. *Journal of Chemical Theory and Computation*, **2013**, 9, 4692-9	6.4	28
49	Investigating Differences in Gas-Phase Conformations of 25-Hydroxyvitamin D3 Sodiated Epimers using Ion Mobility-Mass Spectrometry and Theoretical Modeling. *Journal of the American Society for Mass Spectrometry*, **2017**, 28, 1497-1505	3.5	27

48	NEXMD Software Package for Nonadiabatic Excited State Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2020**, 16, 5771-5783	6.4	27
47	Interpretation of pH-activity profiles for acid-base catalysis from molecular simulations. *Biochemistry*, **2015**, 54, 1307-13	3.2	27
46	Conformational disorder in energy transfer: beyond Förster theory. *Physical Chemistry Chemical Physics*, **2013**, 15, 9245-56	3.6	27
45	Hydrophobic effect drives oxygen uptake in myoglobin via histidine E7. *Journal of Biological Chemistry*, **2013**, 288, 6754-62	5.4	26
44	Enhancement in Organic Photovoltaic Efficiency through the Synergistic Interplay of Molecular Donor Hydrogen Bonding and π-Stacking. *Advanced Functional Materials*, **2015**, 25, 5166-5177	15.6	25
43	Underlying thermodynamics of pH-dependent allostery. *Journal of Physical Chemistry B*, **2014**, 118, 12818-26	3.4	23
42	Ultrafast electronic energy relaxation in a conjugated dendrimer leading to inter-branch energy redistribution. *Physical Chemistry Chemical Physics*, **2016**, 18, 25080-25089	3.6	20
41	Outsmarting Quantum Chemistry Through Transfer Learning		20
40	Structural Study of a Flexible Active Site Loop in Human Indoleamine 2,3-Dioxygenase and Its Functional Implications. *Biochemistry*, **2016**, 55, 2785-93	3.2	20
39	Signature of nonadiabatic coupling in excited-state vibrational modes. *Journal of Physical Chemistry A*, **2014**, 118, 10372-9	2.8	19
38	A Coupled Ionization-Conformational Equilibrium Is Required To Understand the Properties of Ionizable Residues in the Hydrophobic Interior of Staphylococcal Nuclease. *Journal of the American Chemical Society*, **2018**, 140, 1639-1648	16.4	16
37	AM1 Specific Reaction Parameters for Reactions of Hydroxide Ion with Halomethanes in Complex Environments: Development and Testing. *Journal of Chemical Theory and Computation*, **2013**, 9, 4470-80	6.4	15
36	Towards chemical accuracy for alchemical free energy calculations with hybrid physics-based machine learning / molecular mechanics potentials		15
35	Enzyme dynamics and catalysis in the mechanism of DNA polymerase. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	14
34	Improving Efficiency in SMD Simulations Through a Hybrid Differential Relaxation Algorithm. *Journal of Chemical Theory and Computation*, **2014**, 10, 4609-17	6.4	12
33	Oxygen diffusion pathways in a cofactor-independent dioxygenase. *Chemical Science*, **2015**, 6, 6341-6348	9.4	12
32	A Multiscale Treatment of Angeli's Salt Decomposition. *Journal of Chemical Theory and Computation*, **2009**, 5, 37-46	6.4	11
31	Redox potential replica exchange molecular dynamics at constant pH in AMBER: Implementation and validation. *Journal of Chemical Physics*, **2018**, 149, 072338	3.9	10

30	Coarse-Grained Simulations of Heme Proteins: Validation and Study of Large Conformational Transitions. *Journal of Chemical Theory and Computation*, **2016**, 12, 3390-7	6.4	8
29	The generalized Boltzmann distribution is the only distribution in which the Gibbs-Shannon entropy equals the thermodynamic entropy. *Journal of Chemical Physics*, **2019**, 151, 034113	3.9	8
28	Electronic Excited State Specific IR Spectra for Phenylene Ethynylene Dendrimer Building Blocks. *Journal of Physical Chemistry C*, **2013**, 117, 26517-26528	3.8	8
27	Energy transfer and spatial scrambling of an exciton in a conjugated dendrimer. *Physical Chemistry Chemical Physics*, **2018**, 20, 29648-29660	3.6	8
26	Probing the Structures of Solvent-Complexed Ions Formed in Electrospray Ionization Using Cryogenic Infrared Photodissociation Spectroscopy. *Journal of Physical Chemistry A*, **2018**, 122, 7427-7436	2.8	7
25	Theoretical Insights into the Reaction and Inhibition Mechanism of Metal-Independent Retaining Glycosyltransferase Responsible for Mycothiol Biosynthesis. *Journal of Physical Chemistry B*, **2017**, 121, 471-478	3.4	6
24	Fast Implementation of the Nudged Elastic Band Method in AMBER. *Journal of Chemical Theory and Computation*, **2019**, 15, 4699-4707	6.4	5
23	Unraveling Direct and Indirect Energy Transfer Pathways in a Light-Harvesting Dendrimer. *Journal of Physical Chemistry C*, **2020**, 124, 22383-22391	3.8	5
22	Interactively Applying the Variational Method to the Dihydrogen Molecule: Exploring Bonding and Antibonding. *Journal of Chemical Education*, **2016**, 93, 1578-1585	2.4	5
21	Investigating Saccharomyces cerevisiae alkene reductase OYE 3 by substrate profiling, X-ray crystallography and computational methods. *Catalysis Science and Technology*, **2018**, 8, 5003-5016	5.5	5
20	Cation-Dependent Conformations in 25-Hydroxyvitamin D3-Cation Adducts Measured by Ion Mobility-Mass Spectrometry and Theoretical Modeling. *International Journal of Mass Spectrometry*, **2018**, 432, 1-8	1.9	4
19	pH-Dependent Conformational Changes Due to Ionizable Residues in a Hydrophobic Protein Interior: The Study of L25K and L125K Variants of SNase. *Journal of Physical Chemistry B*, **2019**, 123, 5742-5754	3.4	4
18	Steered molecular dynamic simulations reveal Marfan syndrome mutations disrupt fibrillin-1 cbEGF domain mechanosensitive calcium binding. *Scientific Reports*, **2020**, 10, 16844	4.9	4
17	Applicability of fluorescence-based sensors to the determination of kinetic parameters for O□n oxygenases. *Analytical Biochemistry*, **2015**, 475, 53-5	3.1	3
16	On the analysis and comparison of conformer-specific essential dynamics upon ligand binding to a protein. *Journal of Chemical Physics*, **2015**, 142, 245101	3.9	3
15	Exploring Coupled Redox and pH Processes with a Force-Field-Based Approach: Applications to Five Different Systems. *Journal of the American Chemical Society*, **2020**, 142, 3823-3835	16.4	3
14	Using distances between □carbons to predict protein structure. *International Journal of Quantum Chemistry*, **2008**, 108, 2782-2792	2.1	3
13	Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning		3

List of Publications

12	Exploring the concerted mechanistic pathway for HIV-1 PR-substrate revealed by umbrella sampling simulation. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-12	3.6	3
11	Multidimensional Replica Exchange Simulations for Efficient Constant pH and Redox Potential Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2019**, 15, 871-881	6.4	3
10	Axially Chiral Cannabinols: A New Platform for Cannabinoid-Inspired Drug Discovery. *ChemMedChem*, **2020**, 15, 728-732	3.7	2
9	Using the Rosetta algorithm and selected inter-residue distances to predict protein structure. *International Journal of Quantum Chemistry*, **2008**, 108, 2793-2802	2.1	2
8	Extending the Applicability of the ANI Deep Learning Molecular Potential to Sulfur and Halogens		2
7	pH-Dependent Conformational Changes Lead to a Highly Shifted p for a Buried Glutamic Acid Mutant of SNase. *Journal of Physical Chemistry B*, **2020**, 124, 11072-11080	3.4	2
6	The density-of-States and equilibrium charge dynamics of redox-active switches. *Electrochimica Acta*, **2021**, 387, 138410	6.7	2
5	Retraction of "Rationalizing the pH-Activity Response of Glycinamide Ribonucleotide Transformylase through Computational Methods". *Journal of Physical Chemistry B*, **2020**, 124, 5091	3.4	1
4	Folding and Dynamics Are Strongly pH-Dependent in a Psychrophile Frataxin. *Journal of Physical Chemistry B*, **2019**, 123, 7676-7686	3.4	1
3	Construction of vicinal 4°/3°-carbons reductive Cope rearrangement.. *Chemical Science*, **2022**, 13, 1951-1956	9.4	1
2	pH Effects and Cooperativity among Key Titratable Residues for Glycinamide Ribonucleotide Transformylase. *Journal of Physical Chemistry B*, **2021**, 125, 9168-9185	3.4	0
1	The any particle molecular orbital/molecular mechanics approach. *Journal of Molecular Modeling*, **2019**, 25, 316	2	