Adrian E Roitberg

List of Publications by Year
in descending order

101 papers	17,836 citations	50276 46 h-index	30922 102 g-index
113 all docs	113 docs citations	113 times ranked	19323 citing authors

#	Article	IF	Citations
1	Exploring the concerted mechanistic pathway for HIV-1 PRâ€"substrate revealed by umbrella sampling simulation. Journal of Biomolecular Structure and Dynamics, 2022, 40, 1736-1747.	3.5	6
2	Construction of vicinal 4Â°/3Â°-carbonsviareductive Cope rearrangement. Chemical Science, 2022, 13, 1951-1956.	7.4	4
3	Development and Evaluation of Geometry Optimization Algorithms in Conjunction with ANI Potentials. Journal of Chemical Theory and Computation, 2022, 18, 978-991.	5.3	2
4	Anticancer Agents Derived from Cyclic Thiosulfonates: Structureâ€Reactivity and Structureâ€Activity Relationships. ChemMedChem, 2022, 17, .	3.2	1
5	Diastereoselective Indole-Dearomative Cope Rearrangements by Compounding Minor Driving Forces. Organic Letters, 2022, 24, 3726-3730.	4.6	6
6	pH Effects and Cooperativity among Key Titratable Residues for Escherichia coli Glycinamide Ribonucleotide Transformylase. Journal of Physical Chemistry B, 2021, 125, 9168-9185.	2.6	2
7	The density-of-States and equilibrium charge dynamics of redox-active switches. Electrochimica Acta, 2021, 387, 138410.	5.2	8
8	Steered molecular dynamic simulations reveal Marfan syndrome mutations disrupt fibrillin-1 cbEGF domain mechanosensitive calcium binding. Scientific Reports, 2020, 10, 16844.	3.3	8
9	Unraveling Direct and Indirect Energy Transfer Pathways in a Light-Harvesting Dendrimer. Journal of Physical Chemistry C, 2020, 124, 22383-22391.	3.1	12
10	The ANI-1ccx and ANI-1x data sets, coupled-cluster and density functional theory properties for molecules. Scientific Data, 2020, 7, 134.	5.3	104
11	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.	5.4	143
12	Extending the Applicability of the ANI Deep Learning Molecular Potential to Sulfur and Halogens. Journal of Chemical Theory and Computation, 2020, 16, 4192-4202.	5.3	160
13	NEXMD Software Package for Nonadiabatic Excited State Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 5771-5783.	5.3	56
14	Non-adiabatic Excited-State Molecular Dynamics: Theory and Applications for Modeling Photophysics in Extended Molecular Materials. Chemical Reviews, 2020, 120, 2215-2287.	47.7	231
15	Axially Chiral Cannabinols: A New Platform for Cannabinoidâ€Inspired Drug Discovery. ChemMedChem, 2020, 15, 728-732.	3.2	6
16	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.	13.7	15
17	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	38.1	427
18	pH-Dependent Conformational Changes Lead to a Highly Shifted pK_a for a Buried Glutamic Acid Mutant of SNase. Journal of Physical Chemistry B, 2020, 124, 11072-11080.	2.6	6

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19	Folding and Dynamics Are Strongly pH-Dependent in a Psychrophile Frataxin. Journal of Physical Chemistry B, 2019, 123, 7676-7686.	2.6	2
20	Fast Implementation of the Nudged Elastic Band Method in AMBER. Journal of Chemical Theory and Computation, 2019, 15, 4699-4707.	5.3	12
21	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.	3.0	20
22	Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning. Nature Communications, 2019, 10, 2903.	12.8	399
23	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.	2.6	8
24	The any particle molecular orbital/molecular mechanics approach. Journal of Molecular Modeling, 2019, 25, 316.	1.8	1
25	Multidimensional Replica Exchange Simulations for Efficient Constant pH and Redox Potential Molecular Dynamics. Journal of Chemical Theory and Computation, 2019, 15, 871-881.	5.3	3
26	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.	13.7	22
27	Energy transfer and spatial scrambling of an exciton in a conjugated dendrimer. Physical Chemistry Chemical Physics, 2018, 20, 29648-29660.	2.8	15
28	Transforming Computational Drug Discovery with Machine Learning and AI. ACS Medicinal Chemistry Letters, 2018, 9, 1065-1069.	2.8	70
29	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
30	Investigating Saccharomyces cerevisiae alkene reductase OYE 3 by substrate profiling, X-ray crystallography and computational methods. Catalysis Science and Technology, 2018, 8, 5003-5016.	4.1	9
31	Less is more: Sampling chemical space with active learning. Journal of Chemical Physics, 2018, 148, 241733.	3.0	426
32	Transferable Dynamic Molecular Charge Assignment Using Deep Neural Networks. Journal of Chemical Theory and Computation, 2018, 14, 4687-4698.	5.3	81
33	Discovering a Transferable Charge Assignment Model Using Machine Learning. Journal of Physical Chemistry Letters, 2018, 9, 4495-4501.	4.6	88
34	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.	1.5	9
35	Redox potential replica exchange molecular dynamics at constant pH in AMBER: Implementation and validation. Journal of Chemical Physics, 2018, 149, 072338.	3.0	18
36	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.	2.5	11

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37	Photoexcited Nonadiabatic Dynamics of Solvated Pushâ€"Pull Ï€-Conjugated Oligomers with the NEXMD Software. Journal of Chemical Theory and Computation, 2018, 14, 3955-3966.	5.3	39
38	Coherent exciton-vibrational dynamics and energy transfer in conjugated organics. Nature Communications, 2018, 9, 2316.	12.8	71
39	ANI-1: an extensible neural network potential with DFT accuracy at force field computational cost. Chemical Science, 2017, 8, 3192-3203.	7.4	1,111
40	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.	2.8	36
41	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.	2.8	42
42	Electronic Delocalization, Vibrational Dynamics, and Energy Transfer in Organic Chromophores. Journal of Physical Chemistry Letters, 2017, 8, 3020-3031.	4.6	59
43	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.	2.6	9
44	Structureâ€"Activity Relationships of Benzenesulfonamideâ€Based Inhibitors towards Carbonic Anhydrase Isoform Specificity. ChemBioChem, 2017, 18, 213-222.	2.6	38
45	ANI-1, A data set of 20 million calculated off-equilibrium conformations for organic molecules. Scientific Data, 2017, 4, 170193.	5.3	178
46	Structural Study of a Flexible Active Site Loop in Human Indoleamine 2,3-Dioxygenase and Its Functional Implications. Biochemistry, 2016, 55, 2785-2793.	2.5	21
47	Interactively Applying the Variational Method to the Dihydrogen Molecule: Exploring Bonding and Antibonding. Journal of Chemical Education, 2016, 93, 1578-1585.	2.3	8
48	Ultrafast electronic energy relaxation in a conjugated dendrimer leading to inter-branch energy redistribution. Physical Chemistry Chemical Physics, 2016, 18, 25080-25089.	2.8	29
49	Coarse-Grained Simulations of Heme Proteins: Validation and Study of Large Conformational Transitions. Journal of Chemical Theory and Computation, 2016, 12, 3390-3397.	5.3	10
50	Enhancement in Organic Photovoltaic Efficiency through the Synergistic Interplay of Molecular Donor Hydrogen Bonding and Ï€â€Stacking. Advanced Functional Materials, 2015, 25, 5166-5177.	14.9	27
51	Oxygen diffusion pathways in a cofactor-independent dioxygenase. Chemical Science, 2015, 6, 6341-6348.	7.4	17
52	Interpretation of pHâ€"Activity Profiles for Acidâ€"Base Catalysis from Molecular Simulations. Biochemistry, 2015, 54, 1307-1313.	2.5	33
53	Dynamics of Energy Transfer in a Conjugated Dendrimer Driven by Ultrafast Localization of Excitations. Journal of the American Chemical Society, 2015, 137, 11637-11644.	13.7	50
54	Long-Time-Step Molecular Dynamics through Hydrogen Mass Repartitioning. Journal of Chemical Theory and Computation, 2015, 11, 1864-1874.	5.3	896

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55	Applicability of fluorescence-based sensors to the determination of kinetic parameters for O2 in oxygenases. Analytical Biochemistry, 2015, 475, 53-55.	2.4	3
56	On the analysis and comparison of conformer-specific essential dynamics upon ligand binding to a protein. Journal of Chemical Physics, 2015, 142, 245101.	3.0	4
57	Nonadiabatic Excited-State Molecular Dynamics: Modeling Photophysics in Organic Conjugated Materials. Accounts of Chemical Research, 2014, 47, 1155-1164.	15.6	201
58	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, 12577-12585.	2.6	41
59	Underlying Thermodynamics of pH-Dependent Allostery. Journal of Physical Chemistry B, 2014, 118, 12818-12826.	2.6	26
60	Improving Efficiency in SMD Simulations Through a Hybrid Differential Relaxation Algorithm. Journal of Chemical Theory and Computation, 2014, 10, 4609-4617.	5.3	14
61	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
62	Signature of Nonadiabatic Coupling in Excited-State Vibrational Modes. Journal of Physical Chemistry A, 2014, 118, 10372-10379.	2.5	23
63	Multidimensional Replica Exchange Molecular Dynamics Yields a Converged Ensemble of an RNA Tetranucleotide. Journal of Chemical Theory and Computation, 2014, 10, 492-499.	5.3	120
64	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.	2.6	53
65	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, 4470-4480.	5.3	15
66	Electronic Excited State Specific IR Spectra for Phenylene Ethynylene Dendrimer Building Blocks. Journal of Physical Chemistry C, 2013, 117, 26517-26528.	3.1	8
67	Nonadiabatic excited-state molecular dynamics: Treatment of electronic decoherence. Journal of Chemical Physics, 2013, 138, 224111.	3.0	127
68	Optimization of Umbrella Sampling Replica Exchange Molecular Dynamics by Replica Positioning. Journal of Chemical Theory and Computation, 2013, 9, 4692-4699.	5.3	33
69	Hydrophobic Effect Drives Oxygen Uptake in Myoglobin via Histidine E7. Journal of Biological Chemistry, 2013, 288, 6754-6762.	3.4	28
70	Conformational disorder in energy transfer: beyond FÃ¶rster theory. Physical Chemistry Chemical Physics, 2013, 15, 9245.	2.8	33
71	pH-Dependent Conformational Changes in Proteins and Their Effect on Experimental pKas: The Case of Nitrophorin 4. PLoS Computational Biology, 2012, 8, e1002761.	3.2	110
72	Shishiodoshi unidirectional energy transfer mechanism in phenylene ethynylene dendrimers. Journal of Chemical Physics, 2012, 137, 22A526.	3.0	56

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73	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, 4393-4404.	5.3	91
74	Analysis of State-Specific Vibrations Coupled to the Unidirectional Energy Transfer in Conjugated Dendrimers. Journal of Physical Chemistry A, 2012, 116, 9802-9810.	2.5	50
75	pH-Replica Exchange Molecular Dynamics in Proteins Using a Discrete Protonation Method. Journal of Physical Chemistry B, 2012, 116, 8805-8811.	2.6	43
76	Identification of unavoided crossings in nonadiabatic photoexcited dynamics involving multiple electronic states in polyatomic conjugated molecules. Journal of Chemical Physics, 2012, 137, 014512.	3.0	175
77	Nonadiabatic excited-state molecular dynamics: Numerical tests of convergence and parameters. Journal of Chemical Physics, 2012, 136, 054108.	3.0	84
78	Enzyme dynamics and catalysis in the mechanism of DNA polymerase. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	16
79	MMPBSA.py: An Efficient Program for End-State Free Energy Calculations. Journal of Chemical Theory and Computation, 2012, 8, 3314-3321.	5.3	2,891
80	Nonadiabatic Excited-State Molecular Dynamics Modeling of Photoinduced Dynamics in Conjugated Molecules. Journal of Physical Chemistry B, 2011, 115, 5402-5414.	2.6	172
81	Computing Alchemical Free Energy Differences with Hamiltonian Replica Exchange Molecular Dynamics (H-REMD) Simulations. Journal of Chemical Theory and Computation, 2011, 7, 2721-2727.	5.3	78
82	Modeling of Non-Adiabatic Photoinduced Dynamics and Energy Transfer in Conjugated Molecules. , 2010, , .		0
83	Electronic Spectra of the Nanostar Dendrimer: Theory and Experiment. Journal of Physical Chemistry C, 2010, 114, 20702-20712.	3.1	35
84	Unidirectional Energy Transfer in Conjugated Molecules: The Crucial Role of High-Frequency Câ‰¡C Bonds. Journal of Physical Chemistry Letters, 2010, 1, 2699-2704.	4.6	59
85	Exchange Often and Properly in Replica Exchange Molecular Dynamics. Journal of Chemical Theory and Computation, 2010, 6, 2804-2808.	5.3	106
86	Constant pH Replica Exchange Molecular Dynamics in Biomolecules Using a Discrete Protonation Model. Journal of Chemical Theory and Computation, 2010, 6, 1401-1412.	5.3	96
87	Bad Seeds Sprout Perilous Dynamics: Stochastic Thermostat Induced Trajectory Synchronization in Biomolecules. Journal of Chemical Theory and Computation, 2009, 5, 1624-1631.	5.3	170
88	Nonadiabatic Molecular Dynamics Simulations of the Energy Transfer between Building Blocks in a Phenylene Ethynylene Dendrimer. Journal of Physical Chemistry A, 2009, 113, 7535-7542.	2.5	76
89	A Multiscale Treatment of Angeliâ€™s Salt Decomposition. Journal of Chemical Theory and Computation, 2009, 5, 37-46.	5.3	12
90	Using the Rosetta algorithm and selected interâ€residue distances to predict protein structure. International Journal of Quantum Chemistry, 2008, 108, 2793-2802.	2.0	2

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91	Using distances between Î±â€carbons to predict protein structure. International Journal of Quantum Chemistry, 2008, 108, 2782-2792.	2.0	4
92	Exchange frequency in replica exchange molecular dynamics. Journal of Chemical Physics, 2008, 128, 024103.	3.0	119
93	Coupling of Replica Exchange Simulations to a Non-Boltzmann Structure Reservoir. Journal of Physical Chemistry B, 2007, 111, 2415-2418.	2.6	80
94	Implementation of the SCC-DFTB Method for Hybrid QM/MM Simulations within the Amber Molecular Dynamics Packageâ€. Journal of Physical Chemistry A, 2007, 111, 5655-5664.	2.5	213
95	The Catalytic Mechanism of Peptidylglycine Î±-Hydroxylating Monooxygenase Investigated by Computer Simulation. Journal of the American Chemical Society, 2006, 128, 12817-12828.	13.7	137
96	Comparison of multiple Amber force fields and development of improved protein backbone parameters. Proteins: Structure, Function and Bioinformatics, 2006, 65, 712-725.	2.6	6,049
97	Free Energy Calculations with Non-Equilibrium Methods: Applications of the Jarzynski Relationship. Theoretical Chemistry Accounts, 2006, 116, 338-346.	1.4	79
98	Energy Transfer in the Nanostar:â€‰ The Role of Coulombic Coupling and Dynamics. Journal of Physical Chemistry B, 2005, 109, 11512-11519.	2.6	52
99	A DFT-Based QM-MM Approach Designed for the Treatment of Large Molecular Systems:Â Application to Chorismate Mutase. Journal of Physical Chemistry B, 2003, 107, 13728-13736.	2.6	116
100	Solvent-induced symmetry breaking of nitrate ion in aqueous clusters: A quantum-classical simulation study. Journal of Chemical Physics, 2002, 117, 2718-2725.	3.0	46
101	Mo/llerâ€“Plesset perturbation theory applied to vibrational problems. Journal of Chemical Physics, 1996, 105, 11261-11267.	3.0	227