

Adrian E Roitberg

List of Publications by Year in descending order

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101
papers

17,836
citations

57681

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h-index

35168

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113
all docs

113
docs citations

113
times ranked

21671
citing authors

#	ARTICLE	IF	CITATIONS
1	Exploring the concerted mechanistic pathway for HIV-1 PR substrate revealed by umbrella sampling simulation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 1736-1747.	2.0	6
2	Construction of vicinal 4 ^Å /3 ^Å -carbons via reductive Cope rearrangement. <i>Chemical Science</i> , 2022, 13, 1951-1956.	3.7	4
3	Development and Evaluation of Geometry Optimization Algorithms in Conjunction with ANI Potentials. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 978-991.	2.3	2
4	Anticancer Agents Derived from Cyclic Thiosulfonates: Structure-Reactivity and Structure-Activity Relationships. <i>ChemMedChem</i> , 2022, 17, .	1.6	1
5	Diastereoselective Indole-Dearomative Cope Rearrangements by Compounding Minor Driving Forces. <i>Organic Letters</i> , 2022, 24, 3726-3730.	2.4	6
6	pH Effects and Cooperativity among Key Titratable Residues for Escherichia coli Glycinamide Ribonucleotide Transformylase. <i>Journal of Physical Chemistry B</i> , 2021, 125, 9168-9185.	1.2	2
7	The density-of-States and equilibrium charge dynamics of redox-active switches. <i>Electrochimica Acta</i> , 2021, 387, 138410.	2.6	8
8	Steered molecular dynamic simulations reveal Marfan syndrome mutations disrupt fibrillin-1 cbEGF domain mechanosensitive calcium binding. <i>Scientific Reports</i> , 2020, 10, 16844.	1.6	8
9	Unraveling Direct and Indirect Energy Transfer Pathways in a Light-Harvesting Dendrimer. <i>Journal of Physical Chemistry C</i> , 2020, 124, 22383-22391.	1.5	12
10	The ANI-1ccx and ANI-1x data sets, coupled-cluster and density functional theory properties for molecules. <i>Scientific Data</i> , 2020, 7, 134.	2.4	104
11	TorchANI: A Free and Open Source PyTorch-Based Deep Learning Implementation of the ANI Neural Network Potentials. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3408-3415.	2.5	143
12	Extending the Applicability of the ANI Deep Learning Molecular Potential to Sulfur and Halogens. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4192-4202.	2.3	160
13	NEXMD Software Package for Nonadiabatic Excited State Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 5771-5783.	2.3	56
14	Non-adiabatic Excited-State Molecular Dynamics: Theory and Applications for Modeling Photophysics in Extended Molecular Materials. <i>Chemical Reviews</i> , 2020, 120, 2215-2287.	23.0	231
15	Axially Chiral Cannabinoids: A New Platform for Cannabinoid-Inspired Drug Discovery. <i>ChemMedChem</i> , 2020, 15, 728-732.	1.6	6
16	Exploring Coupled Redox and pH Processes with a Force-Field-Based Approach: Applications to Five Different Systems. <i>Journal of the American Chemical Society</i> , 2020, 142, 3823-3835.	6.6	15
17	QSAR without borders. <i>Chemical Society Reviews</i> , 2020, 49, 3525-3564.	18.7	427
18	pH-Dependent Conformational Changes Lead to a Highly Shifted pK _a for a Buried Glutamic Acid Mutant of SNase. <i>Journal of Physical Chemistry B</i> , 2020, 124, 11072-11080.	1.2	6

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19	Folding and Dynamics Are Strongly pH-Dependent in a Psychrophile Frataxin. <i>Journal of Physical Chemistry B</i> , 2019, 123, 7676-7686.	1.2	2
20	Fast Implementation of the Nudged Elastic Band Method in AMBER. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4699-4707.	2.3	12
21	The generalized Boltzmann distribution is the only distribution in which the Gibbs-Shannon entropy equals the thermodynamic entropy. <i>Journal of Chemical Physics</i> , 2019, 151, 034113.	1.2	20
22	Approaching coupled cluster accuracy with a general-purpose neural network potential through transfer learning. <i>Nature Communications</i> , 2019, 10, 2903.	5.8	399
23	pH-Dependent Conformational Changes Due to Ionizable Residues in a Hydrophobic Protein Interior: The Study of L25K and L125K Variants of SNase. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5742-5754.	1.2	8
24	The any particle molecular orbital/molecular mechanics approach. <i>Journal of Molecular Modeling</i> , 2019, 25, 316.	0.8	1
25	Multidimensional Replica Exchange Simulations for Efficient Constant pH and Redox Potential Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 871-881.	2.3	3
26	A Coupled Ionization-Conformational Equilibrium Is Required To Understand the Properties of Ionizable Residues in the Hydrophobic Interior of Staphylococcal Nuclease. <i>Journal of the American Chemical Society</i> , 2018, 140, 1639-1648.	6.6	22
27	Energy transfer and spatial scrambling of an exciton in a conjugated dendrimer. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 29648-29660.	1.3	15
28	Transforming Computational Drug Discovery with Machine Learning and AI. <i>ACS Medicinal Chemistry Letters</i> , 2018, 9, 1065-1069.	1.3	70
29	GPU-Accelerated Molecular Dynamics and Free Energy Methods in Amber18: Performance Enhancements and New Features. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 2043-2050.	2.5	293
30	Investigating <i>Saccharomyces cerevisiae</i> alkene reductase OYE 3 by substrate profiling, X-ray crystallography and computational methods. <i>Catalysis Science and Technology</i> , 2018, 8, 5003-5016.	2.1	9
31	Less is more: Sampling chemical space with active learning. <i>Journal of Chemical Physics</i> , 2018, 148, 241733.	1.2	426
32	Transferable Dynamic Molecular Charge Assignment Using Deep Neural Networks. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4687-4698.	2.3	81
33	Discovering a Transferable Charge Assignment Model Using Machine Learning. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 4495-4501.	2.1	88
34	Cation-dependent conformations in 25-hydroxyvitamin D3-cation adducts measured by ion mobility-mass spectrometry and theoretical modeling. <i>International Journal of Mass Spectrometry</i> , 2018, 432, 1-8.	0.7	9
35	Redox potential replica exchange molecular dynamics at constant pH in AMBER: Implementation and validation. <i>Journal of Chemical Physics</i> , 2018, 149, 072338.	1.2	18
36	Probing the Structures of Solvent-Complexed Ions Formed in Electrospray Ionization Using Cryogenic Infrared Photodissociation Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2018, 122, 7427-7436.	1.1	11

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37	Photoexcited Nonadiabatic Dynamics of Solvated Push-Pull π -Conjugated Oligomers with the NEXMD Software. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3955-3966.	2.3	39
38	Coherent exciton-vibrational dynamics and energy transfer in conjugated organics. <i>Nature Communications</i> , 2018, 9, 2316.	5.8	71
39	ANI-1: an extensible neural network potential with DFT accuracy at force field computational cost. <i>Chemical Science</i> , 2017, 8, 3192-3203.	3.7	1,111
40	Investigating Differences in Gas-Phase Conformations of 25-Hydroxyvitamin D3 Sodiated Epimers using Ion Mobility-Mass Spectrometry and Theoretical Modeling. <i>Journal of the American Society for Mass Spectrometry</i> , 2017, 28, 1497-1505.	1.2	36
41	Experimental and Theoretical Investigation of Sodiated Multimers of Steroid Epimers with Ion Mobility-Mass Spectrometry. <i>Journal of the American Society for Mass Spectrometry</i> , 2017, 28, 323-331.	1.2	42
42	Electronic Delocalization, Vibrational Dynamics, and Energy Transfer in Organic Chromophores. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3020-3031.	2.1	59
43	Theoretical Insights into the Reaction and Inhibition Mechanism of Metal-Independent Retaining Glycosyltransferase Responsible for Mycothiol Biosynthesis. <i>Journal of Physical Chemistry B</i> , 2017, 121, 471-478.	1.2	9
44	Structure-Activity Relationships of Benzenesulfonamide-Based Inhibitors towards Carbonic Anhydrase Isoform Specificity. <i>ChemBioChem</i> , 2017, 18, 213-222.	1.3	38
45	ANI-1, A data set of 20 million calculated off-equilibrium conformations for organic molecules. <i>Scientific Data</i> , 2017, 4, 170193.	2.4	178
46	Structural Study of a Flexible Active Site Loop in Human Indoleamine 2,3-Dioxygenase and Its Functional Implications. <i>Biochemistry</i> , 2016, 55, 2785-2793.	1.2	21
47	Interactively Applying the Variational Method to the Dihydrogen Molecule: Exploring Bonding and Antibonding. <i>Journal of Chemical Education</i> , 2016, 93, 1578-1585.	1.1	8
48	Ultrafast electronic energy relaxation in a conjugated dendrimer leading to inter-branch energy redistribution. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 25080-25089.	1.3	29
49	Coarse-Grained Simulations of Heme Proteins: Validation and Study of Large Conformational Transitions. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3390-3397.	2.3	10
50	Enhancement in Organic Photovoltaic Efficiency through the Synergistic Interplay of Molecular Donor Hydrogen Bonding and π -Stacking. <i>Advanced Functional Materials</i> , 2015, 25, 5166-5177.	7.8	27
51	Oxygen diffusion pathways in a cofactor-independent dioxygenase. <i>Chemical Science</i> , 2015, 6, 6341-6348.	3.7	17
52	Interpretation of pH-Activity Profiles for Acid-Base Catalysis from Molecular Simulations. <i>Biochemistry</i> , 2015, 54, 1307-1313.	1.2	33
53	Dynamics of Energy Transfer in a Conjugated Dendrimer Driven by Ultrafast Localization of Excitations. <i>Journal of the American Chemical Society</i> , 2015, 137, 11637-11644.	6.6	50
54	Long-Time-Step Molecular Dynamics through Hydrogen Mass Repartitioning. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1864-1874.	2.3	896

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55	Applicability of fluorescence-based sensors to the determination of kinetic parameters for O ₂ in oxygenases. <i>Analytical Biochemistry</i> , 2015, 475, 53-55.	1.1	3
56	On the analysis and comparison of conformer-specific essential dynamics upon ligand binding to a protein. <i>Journal of Chemical Physics</i> , 2015, 142, 245101.	1.2	4
57	Nonadiabatic Excited-State Molecular Dynamics: Modeling Photophysics in Organic Conjugated Materials. <i>Accounts of Chemical Research</i> , 2014, 47, 1155-1164.	7.6	201
58	pH-REMD Simulations Indicate That the Catalytic Aspartates of HIV-1 Protease Exist Primarily in a Monoprotonated State. <i>Journal of Physical Chemistry B</i> , 2014, 118, 12577-12585.	1.2	41
59	Underlying Thermodynamics of pH-Dependent Allostery. <i>Journal of Physical Chemistry B</i> , 2014, 118, 12818-12826.	1.2	26
60	Improving Efficiency in SMD Simulations Through a Hybrid Differential Relaxation Algorithm. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 4609-4617.	2.3	14
61	Constant pH Replica Exchange Molecular Dynamics in Explicit Solvent Using Discrete Protonation States: Implementation, Testing, and Validation. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1341-1352.	2.3	210
62	Signature of Nonadiabatic Coupling in Excited-State Vibrational Modes. <i>Journal of Physical Chemistry A</i> , 2014, 118, 10372-10379.	1.1	23
63	Multidimensional Replica Exchange Molecular Dynamics Yields a Converged Ensemble of an RNA Tetranucleotide. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 492-499.	2.3	120
64	Artifacts due to trivial unavoided crossings in the modeling of photoinduced energy transfer dynamics in extended conjugated molecules. <i>Chemical Physics Letters</i> , 2013, 590, 208-213.	1.2	53
65	AM1 Specific Reaction Parameters for Reactions of Hydroxide Ion with Halomethanes in Complex Environments: Development and Testing. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4470-4480.	2.3	15
66	Electronic Excited State Specific IR Spectra for Phenylene Ethynylene Dendrimer Building Blocks. <i>Journal of Physical Chemistry C</i> , 2013, 117, 26517-26528.	1.5	8
67	Nonadiabatic excited-state molecular dynamics: Treatment of electronic decoherence. <i>Journal of Chemical Physics</i> , 2013, 138, 224111.	1.2	127
68	Optimization of Umbrella Sampling Replica Exchange Molecular Dynamics by Replica Positioning. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4692-4699.	2.3	33
69	Hydrophobic Effect Drives Oxygen Uptake in Myoglobin via Histidine E7. <i>Journal of Biological Chemistry</i> , 2013, 288, 6754-6762.	1.6	28
70	Conformational disorder in energy transfer: beyond Förster theory. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 9245.	1.3	33
71	pH-Dependent Conformational Changes in Proteins and Their Effect on Experimental pK _a s: The Case of Nitrophorin 4. <i>PLoS Computational Biology</i> , 2012, 8, e1002761.	1.5	110
72	Shishiodoshi unidirectional energy transfer mechanism in phenylene ethynylene dendrimers. <i>Journal of Chemical Physics</i> , 2012, 137, 22A526.	1.2	56

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73	Enhancing Conformation and Protonation State Sampling of Hen Egg White Lysozyme Using pH Replica Exchange Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4393-4404.	2.3	91
74	Analysis of State-Specific Vibrations Coupled to the Unidirectional Energy Transfer in Conjugated Dendrimers. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9802-9810.	1.1	50
75	pH-Replica Exchange Molecular Dynamics in Proteins Using a Discrete Protonation Method. <i>Journal of Physical Chemistry B</i> , 2012, 116, 8805-8811.	1.2	43
76	Identification of unavoided crossings in nonadiabatic photoexcited dynamics involving multiple electronic states in polyatomic conjugated molecules. <i>Journal of Chemical Physics</i> , 2012, 137, 014512.	1.2	175
77	Nonadiabatic excited-state molecular dynamics: Numerical tests of convergence and parameters. <i>Journal of Chemical Physics</i> , 2012, 136, 054108.	1.2	84
78	Enzyme dynamics and catalysis in the mechanism of DNA polymerase. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	16
79	<i>MMPBSA.py</i> : An Efficient Program for End-State Free Energy Calculations. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3314-3321.	2.3	2,891
80	Nonadiabatic Excited-State Molecular Dynamics Modeling of Photoinduced Dynamics in Conjugated Molecules. <i>Journal of Physical Chemistry B</i> , 2011, 115, 5402-5414.	1.2	172
81	Computing Alchemical Free Energy Differences with Hamiltonian Replica Exchange Molecular Dynamics (H-REMD) Simulations. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2721-2727.	2.3	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. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20702-20712.	1.5	35
84	Unidirectional Energy Transfer in Conjugated Molecules: The Crucial Role of High-Frequency C=C Bonds. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 2699-2704.	2.1	59
85	Exchange Often and Properly in Replica Exchange Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 2804-2808.	2.3	106
86	Constant pH Replica Exchange Molecular Dynamics in Biomolecules Using a Discrete Protonation Model. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1401-1412.	2.3	96
87	Bad Seeds Sprout Perilous Dynamics: Stochastic Thermostat Induced Trajectory Synchronization in Biomolecules. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1624-1631.	2.3	170
88	Nonadiabatic Molecular Dynamics Simulations of the Energy Transfer between Building Blocks in a Phenylene Ethynylene Dendrimer. <i>Journal of Physical Chemistry A</i> , 2009, 113, 7535-7542.	1.1	76
89	A Multiscale Treatment of Angeli's Salt Decomposition. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 37-46.	2.3	12
90	Using the Rosetta algorithm and selected inter-residue distances to predict protein structure. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2793-2802.	1.0	2

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91	Using distances between α -carbons to predict protein structure. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 2782-2792.	1.0	4
92	Exchange frequency in replica exchange molecular dynamics. <i>Journal of Chemical Physics</i> , 2008, 128, 024103.	1.2	119
93	Coupling of Replica Exchange Simulations to a Non-Boltzmann Structure Reservoir. <i>Journal of Physical Chemistry B</i> , 2007, 111, 2415-2418.	1.2	80
94	Implementation of the SCC-DFTB Method for Hybrid QM/MM Simulations within the Amber Molecular Dynamics Package. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5655-5664.	1.1	213
95	The Catalytic Mechanism of Peptidylglycine α -Hydroxylating Monooxygenase Investigated by Computer Simulation. <i>Journal of the American Chemical Society</i> , 2006, 128, 12817-12828.	6.6	137
96	Comparison of multiple Amber force fields and development of improved protein backbone parameters. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 65, 712-725.	1.5	6,049
97	Free Energy Calculations with Non-Equilibrium Methods: Applications of the Jarzynski Relationship. <i>Theoretical Chemistry Accounts</i> , 2006, 116, 338-346.	0.5	79
98	Energy Transfer in the Nanostar: The Role of Coulombic Coupling and Dynamics. <i>Journal of Physical Chemistry B</i> , 2005, 109, 11512-11519.	1.2	52
99	A DFT-Based QM-MM Approach Designed for the Treatment of Large Molecular Systems: Application to Chorismate Mutase. <i>Journal of Physical Chemistry B</i> , 2003, 107, 13728-13736.	1.2	116
100	Solvent-induced symmetry breaking of nitrate ion in aqueous clusters: A quantum-classical simulation study. <i>Journal of Chemical Physics</i> , 2002, 117, 2718-2725.	1.2	46
101	Møller-Plesset perturbation theory applied to vibrational problems. <i>Journal of Chemical Physics</i> , 1996, 105, 11261-11267.	1.2	227