Edina Rosta

List of Publications by Year
in descending order

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102	10,370	94269	42291
papers	citations	37 h-index	92 g-index

110	110	110	12348
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Advances in methods and algorithms in a modern quantum chemistry program package. Physical Chemistry Chemical Physics, 2006, 8, 3172-3191.	1.3	2,597
2	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
3	Single-molecule strong coupling at room temperature in plasmonic nanocavities. Nature, 2016, 535, 127-130.	13.7	1,391
4	On the Mechanism of Hydrolysis of Phosphate Monoesters Dianions in Solutions and Proteins. Journal of the American Chemical Society, 2006, 128, 15310-15323.	6.6	191
5	On Possible Pitfalls in ab Initio Quantum Mechanics/Molecular Mechanics Minimization Approaches for Studies of Enzymatic Reactions. Journal of Physical Chemistry B, 2005, 109, 15645-15650.	1.2	164
6	Catalytic Mechanism of RNA Backbone Cleavage by Ribonuclease H from Quantum Mechanics/Molecular Mechanics Simulations. Journal of the American Chemical Society, 2011, 133, 8934-8941.	6.6	164
7	Towards Accurate Ab Initio QM/MM Calculations of Free-Energy Profiles of Enzymatic Reactions. Journal of Physical Chemistry B, 2006, 110, 2934-2941.	1.2	157
8	Free Energies from Dynamic Weighted Histogram Analysis Using Unbiased Markov State Model. Journal of Chemical Theory and Computation, 2015, 11, 276-285.	2.3	116
9	Biomolecular simulations: From dynamics and mechanisms to computational assays of biological activity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1393.	6.2	110
10	Using the Constrained DFT Approach in Generating Diabatic Surfaces and Off Diagonal Empirical Valence Bond Terms for Modeling Reactions in Condensed Phases. Journal of Physical Chemistry B, 2006, 110, 19570-19574.	1.2	108
11	On the Interpretation of the Observed Linear Free Energy Relationship in Phosphate Hydrolysis: A Thorough Computational Study of Phosphate Diester Hydrolysis in Solution. Biochemistry, 2008, 47, 3725-3735.	1.2	103
12	Extending the mirror neuron system model, I. Biological Cybernetics, 2007, 96, 9-38.	0.6	102
13	Two-body zeroth order Hamiltonians in multireference perturbation theory: The APSG reference state. Journal of Chemical Physics, 2002, 116, 878-890.	1.2	100
14	Room-Temperature Optical Picocavities below 1 nm³ Accessing Single-Atom Geometries. Journal of Physical Chemistry Letters, 2018, 9, 7146-7151.	2.1	88
15	Error and efficiency of replica exchange molecular dynamics simulations. Journal of Chemical Physics, 2009, 131, 165102.	1.2	85
16	Cucurbit[7]uril as a Supramolecular Artificial Enzyme for Dielsâ€“Alder Reactions. Angewandte Chemie - International Edition, 2017, 56, 15688-15692.	7.2	84
17	Artificial reaction coordinate â€œtunnelingâ€•in freeâ€energy calculations: The catalytic reaction of RNase H. Journal of Computational Chemistry, 2009, 30, 1634-1641.	1.5	81
18	Thermostat Artifacts in Replica Exchange Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2009, 5, 1393-1399.	2.3	81

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19	Light-Regulated Molecular Trafficking in a Synthetic Water-Soluble Host. Journal of the American Chemical Society, 2016, 138, 5745-5748.	6.6	75
20	Statistically optimal analysis of state-discretized trajectory data from multiple thermodynamic states. Journal of Chemical Physics, 2014, 141, 214106.	1.2	73
21	Structural basis of second-generation HIV integrase inhibitor action and viral resistance. Science, 2020, 367, 806-810.	6.0	73
22	Turning Cucurbit[8]uril into a Supramolecular Nanoreactor for Asymmetric Catalysis. Angewandte Chemie - International Edition, 2015, 54, 13007-13011.	7.2	71
23	Quantum Mechanical/Molecular Mechanical Free Energy Simulations of the Self-Cleavage Reaction in the Hepatitis Delta Virus Ribozyme. Journal of the American Chemical Society, 2014, 136, 1483-1496.	6.6	69
24	A Dynamic and Responsive Host in Action: Lightâ€Controlled Molecular Encapsulation. Angewandte Chemie - International Edition, 2016, 55, 16096-16100.	7.2	62
25	Detecting mid-infrared light by molecular frequency upconversion in dual-wavelength nanoantennas. Science, 2021, 374, 1268-1271.	6.0	61
26	Covalent bond orders and atomic valences from correlated wavefunctions. Chemical Physics Letters, 1999, 299, 1-8.	1.2	60
27	Dynamic Histogram Analysis To Determine Free Energies and Rates from Biased Simulations. Journal of Chemical Theory and Computation, 2017, 13, 6328-6342.	2.3	54
28	Dissecting RAF Inhibitor Resistance by Structure-based Modeling Reveals Ways to Overcome Oncogenic RAS Signaling. Cell Systems, 2018, 7, 161-179.e14.	2.9	53
29	Accelerating QM/MM Free Energy Calculations:Â Representing the Surroundings by an Updated Mean Charge Distribution. Journal of Physical Chemistry B, 2008, 112, 5680-5692.	1.2	52
30	Calcium Inhibition of Ribonuclease H1 Two-Metal Ion Catalysis. Journal of the American Chemical Society, 2014, 136, 3137-3144.	6.6	52
31	Markov Models of Molecular Kinetics. Journal of Chemical Physics, 2019, 151, 190401.	1.2	52
32	Molecular simulations unravel the molecular principles that mediate selective permeability of carboxysome shell protein. Scientific Reports, 2020, 10, 17501.	1.6	52
33	Controlling the structure and photophysics of fluorophore dimers using multiple cucurbit[8]uril clampings. Chemical Science, 2020, 11, 812-825.	3.7	48
34	Direct Evidence for a Peroxide Intermediate and a Reactive Enzymeâ€“Substrateâ€“Dioxygen Configuration in a Cofactorâ€free Oxidase. Angewandte Chemie - International Edition, 2014, 53, 13710-13714.	7.2	43
35	Phosphorylation of RAF Kinase Dimers Drives Conformational Changes that Facilitate Transactivation. Angewandte Chemie - International Edition, 2016, 55, 983-986.	7.2	43
36	Modular supramolecular dimerization of optically tunable extended aryl viologens. Chemical Science, 2019, 10, 8806-8811.	3.7	43

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37	Hostâ€“Guest Chemistry Meets Electrocatalysis: Cucurbit[6]uril on a Au Surface as a Hybrid System in CO₂ Reduction. ACS Catalysis, 2020, 10, 751-761.	5.5	43
38	Theoretical Study of the Mechanism of the Hydride Transfer between Ferredoxinâ€“NADP⁺ Reductase and NADP⁺: The Role of Tyr303. Journal of the American Chemical Society, 2012, 134, 20544-20553.	6.6	40
39	Mechanistic study of an immobilized molecular electrocatalyst by in situ gap-plasmon-assisted spectro-electrochemistry. Nature Catalysis, 2021, 4, 157-163.	16.1	36
40	Insights into functions of the H channel of cytochrome c oxidase from atomistic molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E10339-E10348.	3.3	35
41	Anomalously Large Spectral Shifts near the Quantum Tunnelling Limit in Plasmonic Rulers with Subatomic Resolution. Nano Letters, 2019, 19, 2051-2058.	4.5	35
42	Error and efficiency of simulated tempering simulations. Journal of Chemical Physics, 2010, 132, 034102.	1.2	34
43	Understanding the Mechanism of the Hydrogen Abstraction from Arachidonic Acid Catalyzed by the Human Enzyme 15-Lipoxygenase-2. A Quantum Mechanics/Molecular Mechanics Free Energy Simulation. Journal of Chemical Theory and Computation, 2016, 12, 2079-2090.	2.3	33
44	Structural Characterization of Arginine Fingers: Identification of an Arginine Finger for the Pyrophosphatase dUTPases. Journal of the American Chemical Society, 2016, 138, 15035-15045.	6.6	32
45	On Unjustifiably Misrepresenting the EVB Approach While Simultaneously Adopting It. Journal of Physical Chemistry B, 2009, 113, 10905-10915.	1.2	31
46	Cucurbit[7]uril as a Supramolecular Artificial Enzyme for Dielsâ€“Alder Reactions. Angewandte Chemie, 2017, 129, 15894-15898.	1.6	29
47	Human DHEA sulfation requires direct interaction between PAPS synthase 2 and DHEA sulfotransferase SULT2A1. Journal of Biological Chemistry, 2018, 293, 9724-9735.	1.6	29
48	Cucurbit[8]uril-mediated pseudo[2,3]rotaxanes. Chemical Communications, 2019, 55, 13227-13230.	2.2	29
49	Molecular mechanisms of asymmetric RAF dimer activation. Biochemical Society Transactions, 2014, 42, 784-790.	1.6	28
50	Mutations Decouple Proton Transfer from Phosphate Cleavage in the dUTPase Catalytic Reaction. ACS Catalysis, 2015, 5, 3225-3237.	5.5	28
51	Variational Identification of Markovian Transition States. Physical Review X, 2017, 7, .	2.8	28
52	Inhibiting Analyte Theft in Surface-Enhanced Raman Spectroscopy Substrates: Subnanomolar Quantitative Drug Detection. ACS Sensors, 2019, 4, 2988-2996.	4.0	27
53	Coarse Master Equations for Binding Kinetics of Amyloid Peptide Dimers. Journal of Physical Chemistry Letters, 2016, 7, 2676-2682.	2.1	25
54	Cations in motion: QM/MM studies of the dynamic and electrostatic roles of H+ and Mg2+ ions in enzyme reactions. Current Opinion in Structural Biology, 2020, 61, 198-206.	2.6	24

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55	Origin of Linear Free Energy Relationships: Exploring the Nature of the Off-Diagonal Coupling Elements in S_N2 Reactions. Journal of Chemical Theory and Computation, 2012, 8, 3574-3585.	2.3	23
56	Calculating Kinetic Rates and Membrane Permeability from Biased Simulations. Journal of Physical Chemistry B, 2018, 122, 11571-11578.	1.2	21
57	Turning Cucurbit[8]uril into a Supramolecular Nanoreactor for Asymmetric Catalysis. Angewandte Chemie, 2015, 127, 13199-13203.	1.6	20
58	Smart supramolecular sensing with cucurbit[n]urils: probing hydrogen bonding with SERS. Faraday Discussions, 2017, 205, 505-515.	1.6	20
59	Optical probes of molecules as nano-mechanical switches. Nature Communications, 2020, 11, 5905.	5.8	20
60	Exploring the role of the 5-substituent for the intrinsic fluorescence of 5-aryl and 5-heteroaryl uracil nucleotides: a systematic study. Organic and Biomolecular Chemistry, 2013, 11, 6357.	1.5	19
61	A Dynamic and Responsive Host in Action: Lightâ€Controlled Molecular Encapsulation. Angewandte Chemie, 2016, 128, 16330-16334.	1.6	19
62	A simplified charge projection scheme for long-range electrostatics in ab initio QM/MM calculations. Journal of Chemical Physics, 2021, 154, 024115.	1.2	18
63	Understanding the Molecular Mechanism of the Ala-versus-Gly Concept Controlling the Product Specificity in Reactions Catalyzed by Lipoxygenases: A Combined Molecular Dynamics and QM/MM Study of Coral 8R-Lipoxygenase. ACS Catalysis, 2017, 7, 4854-4866.	5.5	17
64	Mean first passage times in variational coarse graining using Markov state models. Journal of Chemical Physics, 2019, 150, 134107.	1.2	17
65	Position-Dependent Diffusion from Biased Simulations and Markov State Model Analysis. Journal of Chemical Theory and Computation, 2021, 17, 2022-2033.	2.3	17
66	Resolving sub-angstrom ambient motion through reconstruction from vibrational spectra. Nature Communications, 2021, 12, 6759.	5.8	17
67	Peptide dimerization-dissociation rates from replica exchange molecular dynamics. Journal of Chemical Physics, 2017, 147, 152725.	1.2	16
68	Nanoparticle surfactants for kinetically arrested photoactive assemblies to track light-induced electron transfer. Nature Nanotechnology, 2021, 16, 1121-1129.	15.6	16
69	Combined Free-Energy Calculation and Machine Learning Methods for Understanding Ligand Unbinding Kinetics. Journal of Chemical Theory and Computation, 2022, 18, 2543-2555.	2.3	16
70	SARAH Domain-Mediated MST2-RASSF Dimeric Interactions. PLoS Computational Biology, 2016, 12, e1005051.	1.5	15
71	Breaking the Selection Rules of Spin-Forbidden Molecular Absorption in Plasmonic Nanocavities. ACS Photonics, 2020, 7, 2337-2342.	3.2	15
72	Catalytic mechanism of Î±-phosphate attack in dUTPase is revealed by X-ray crystallographic snapshots of distinct intermediates, 31P-NMR spectroscopy and reaction path modelling. Nucleic Acids Research, 2013, 41, 10542-10555.	6.5	14

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73	Modulating the oxidation of cucurbit[n]urils. Organic and Biomolecular Chemistry, 2017, 15, 998-1005.	1.5	14
74	MST2-RASSF proteinâ€“protein interactions through SARAH domains. Briefings in Bioinformatics, 2016, 17, 593-602.	3.2	13
75	Correlation functions, mean first passage times, and the Kemeny constant. Journal of Chemical Physics, 2020, 152, 104108.	1.2	13
76	Optical suppression of energy barriers in single molecule-metal binding. Science Advances, 2022, 8, .	4.7	13
77	Organocatalytic Access to a cis-Cyclopentyl-Î³-amino Acid: An Intriguing Model of Selectivity and Formation of a Stable 10/12-Helix from the Corresponding Î³/Î±-Peptide. Journal of the American Chemical Society, 2020, 142, 1382-1393.	6.6	11
78	The Role of Conserved Residues in the DEDDh Motif: the Proton-Transfer Mechanism of HIV-1 RNase H. ACS Catalysis, 2021, 11, 7915-7927.	5.5	11
79	Geometry and electronic structure of bis(tetrahydridoborato)bis(cyclopentadienyl)zirconium(IV). Journal of Organometallic Chemistry, 1999, 582, 267-272.	0.8	9
80	Divergence from the classical hydroboration reactivity; boron containing materials through a hydroboration cascade of small cyclic dienes. Chemical Science, 2015, 6, 6262-6269.	3.7	8
81	Representation of the QM Subsystem for Long-Range Electrostatic Interaction in Non-Periodic Ab Initio QM/MM Calculations. Molecules, 2018, 23, 2500.	1.7	8
82	Limiting relaxation times from Markov state models. Journal of Chemical Physics, 2018, 149, 072324.	1.2	7
83	Spectroscopic Evidence for Peptide-Bond-Selective Ultraviolet Photodissociation. Journal of Physical Chemistry Letters, 2020, 11, 206-209.	2.1	7
84	Toward Understanding CB[7]-Based Supramolecular Diels-Alder Catalysis. Frontiers in Chemistry, 2020, 8, 587084.	1.8	6
85	Modelling the active SARS-CoV-2 helicase complex as a basis for structure-based inhibitor design. Chemical Science, 2021, 12, 13492-13505.	3.7	6
86	Joint neutron/X-ray crystal structure of a mechanistically relevant complex of perdeuterated urate oxidase and simulations provide insight into the hydration step of catalysis. IUCrJ, 2021, 8, 46-59.	1.0	6
87	THE MIRROR SYSTEM HYPOTHESIS: FROM A MACAQUE-LIKE MIRROR SYSTEM TO IMITATION. , 2006, , .		6
88	Efficient Irreversible Monte Carlo Samplers. Journal of Chemical Theory and Computation, 2020, 16, 2124-2138.	2.3	5
89	Deviation from the anti-Markovnikov rule: a computational study of the regio- and stereoselectivity of diene hydroboration reactions. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	3
90	Gas-phase structures reflect the pain-relief potency of enkephalin peptides. Physical Chemistry Chemical Physics, 2019, 21, 22700-22703.	1.3	3

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91	Combining data integration and molecular dynamics for target identification in Î±-Synuclein-aggregating neurodegenerative diseases: Structural insights on Synaptojanin-1 (Synj1). Computational and Structural Biotechnology Journal, 2020, 18, 1032-1042.	1.9	3
92	Molecular Vibration Explorer: an Online Database and Toolbox for Surface-Enhanced Frequency Conversion and Infrared and Raman Spectroscopy. Journal of Physical Chemistry A, 0, , .	1.1	3
93	Structural Dynamics and Catalytic Mechanism of ATP13A2 (PARK9) from Simulations. Journal of Physical Chemistry B, 2021, 125, 11835-11847.	1.2	2
94	Innentitelbild: A Dynamic and Responsive Host in Action: Light-Controlled Molecular Encapsulation (Angew. Chem. 52/2016). Angewandte Chemie, 2016, 128, 16164-16164.	1.6	0
95	Phosphorylation of RAF Kinase Dimers Drives Conformational Changes that Facilitate Transactivation. Angewandte Chemie, 2016, 128, 995-998.	1.6	0
96	The differential impact of PAPS synthase isoforms on DHEAS may be explained by an isoform-specific interaction of SULT2A1 with PAPSS2, but not PAPSS1. Endocrine Abstracts, 0, , .	0.0	0
97	Deviation from the anti-Markovnikov rule: a computational study of the regio- and stereoselectivity of diene hydroboration reactions. Highlights in Theoretical Chemistry, 2016, , 235-248.	0.0	0
98	1 Host-guest Chemistry Meets Electrocatalysis: Cucurbit[6]uril on a Au Surface as Hybrid System in CO2 Reduction. , 0, , .		0
99	Simulated tempering with irreversible Gibbs sampling techniques. Journal of Chemical Physics, 2020, 153, 214111.	1.2	0
100	Editorial: Experiments and Simulations: A Pas de Deux to Unravel Biological Function. Frontiers in Molecular Biosciences, 2021, 8, 799406.	1.6	0
101	Molecular Screening for Terahertz Detection with Machine-Learning-Based Methods. Physical Review X, 2021, 11, .	2.8	0
102	Host-guest Chemistry Meets Electrocatalysis: Cucurbit[6]uril on a Au Surface as Hybrid System in CO2 Reduction. , 0, , .		0