Edina Rosta

List of Publications by Citations

94 papers	8,352 citations	31 h-index	91 g-index
110 ext. papers	9,451 ext. citations	9 avg, IF	5.68 L-index

#	Paper	IF	Citations
94	Advances in methods and algorithms in a modern quantum chemistry program package. *Physical Chemistry Chemical Physics*, **2006**, 8, 3172-91	3.6	2371
93	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. *Molecular Physics*, **2015**, 113, 184-215	1.7	2068
92	Single-molecule strong coupling at room temperature in plasmonic nanocavities. *Nature*, **2016**, 535, 127-30	38.1	1009
91	On the mechanism of hydrolysis of phosphate monoesters dianions in solutions and proteins. *Journal of the American Chemical Society*, **2006**, 128, 15310-23	16.4	179
90	On possible pitfalls in ab initio quantum mechanics/molecular mechanics minimization approaches for studies of enzymatic reactions. *Journal of Physical Chemistry B*, **2005**, 109, 15645-50	3.4	160
89	Towards accurate ab initio QM/MM calculations of free-energy profiles of enzymatic reactions. *Journal of Physical Chemistry B*, **2006**, 110, 2934-41	3.4	148
88	Catalytic mechanism of RNA backbone cleavage by ribonuclease H from quantum mechanics/molecular mechanics simulations. *Journal of the American Chemical Society*, **2011**, 133, 8934-41	16.4	137
87	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, 19570-4	3.4	99
86	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, 3725-35	3.2	98
85	Extending the mirror neuron system model, I. Audible actions and invisible grasps. *Biological Cybernetics*, **2007**, 96, 9-38	2.8	94
84	Two-body zeroth order Hamiltonians in multireference perturbation theory: The APSG reference state. *Journal of Chemical Physics*, **2002**, 116, 878-890	3.9	94
83	Free energies from dynamic weighted histogram analysis using unbiased Markov state model. *Journal of Chemical Theory and Computation*, **2015**, 11, 276-85	6.4	90
82	Artificial reaction coordinate "tunneling" in free-energy calculations: the catalytic reaction of RNase H. *Journal of Computational Chemistry*, **2009**, 30, 1634-41	3.5	73
81	Thermostat artifacts in replica exchange molecular dynamics simulations. *Journal of Chemical Theory and Computation*, **2009**, 5, 1393-1399	6.4	72
80	Error and efficiency of replica exchange molecular dynamics simulations. *Journal of Chemical Physics*, **2009**, 131, 165102	3.9	70
79	Biomolecular simulations: From dynamics and mechanisms to computational assays of biological activity. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1393	7.9	69
78	Light-Regulated Molecular Trafficking in a Synthetic Water-Soluble Host. *Journal of the American Chemical Society*, **2016**, 138, 5745-8	16.4	63

77	Statistically optimal analysis of state-discretized trajectory data from multiple thermodynamic states. *Journal of Chemical Physics*, **2014**, 141, 214106	3.9	62
76	Turning Cucurbit[8]uril into a Supramolecular Nanoreactor for Asymmetric Catalysis. *Angewandte Chemie - International Edition*, **2015**, 54, 13007-11	16.4	60
75	Room-Temperature Optical Picocavities below 1 nm Accessing Single-Atom Geometries. *Journal of Physical Chemistry Letters*, **2018**, 9, 7146-7151	6.4	59
74	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, 1483-96	16.4	57
73	Cucurbit[7]uril as a Supramolecular Artificial Enzyme for Diels-Alder Reactions. *Angewandte Chemie - International Edition*, **2017**, 56, 15688-15692	16.4	54
72	Covalent bond orders and atomic valences from correlated wavefunctions. *Chemical Physics Letters*, **1999**, 299, 1-8	2.5	53
71	Accelerating QM/MM free energy calculations: representing the surroundings by an updated mean charge distribution. *Journal of Physical Chemistry B*, **2008**, 112, 5680-92	3.4	50
70	A Dynamic and Responsive Host in Action: Light-Controlled Molecular Encapsulation. *Angewandte Chemie - International Edition*, **2016**, 55, 16096-16100	16.4	48
69	Dynamic Histogram Analysis To Determine Free Energies and Rates from Biased Simulations. *Journal of Chemical Theory and Computation*, **2017**, 13, 6328-6342	6.4	42
68	Calcium inhibition of ribonuclease H1 two-metal ion catalysis. *Journal of the American Chemical Society*, **2014**, 136, 3137-44	16.4	40
67	Structural basis of second-generation HIV integrase inhibitor action and viral resistance. *Science*, **2020**, 367, 806-810	33.3	34
66	Phosphorylation of RAF Kinase Dimers Drives Conformational Changes that Facilitate Transactivation. *Angewandte Chemie - International Edition*, **2016**, 55, 983-6	16.4	33
65	Error and efficiency of simulated tempering simulations. *Journal of Chemical Physics*, **2010**, 132, 034102	3.9	33
64	Dissecting RAF Inhibitor Resistance by Structure-based Modeling Reveals Ways to Overcome Oncogenic RAS Signaling. *Cell Systems*, **2018**, 7, 161-179.e14	10.6	32
63	Theoretical study of the mechanism of the hydride transfer between ferredoxin-NADP+ reductase and NADP+: the role of Tyr303. *Journal of the American Chemical Society*, **2012**, 134, 20544-53	16.4	30
62	Modular supramolecular dimerization of optically tunable extended aryl viologens. *Chemical Science*, **2019**, 10, 8806-8811	9.4	29
61	Direct evidence for a peroxide intermediate and a reactive enzyme-substrate-dioxygen configuration in a cofactor-free oxidase. *Angewandte Chemie - International Edition*, **2014**, 53, 13710-4	16.4	28
60	On unjustifiably misrepresenting the EVB approach while simultaneously adopting it. *Journal of Physical Chemistry B*, **2009**, 113, 10905-15	3.4	28

59	Molecular simulations unravel the molecular principles that mediate selective permeability of carboxysome shell protein. *Scientific Reports*, **2020**, 10, 17501	4.9	27
58	Molecular mechanisms of asymmetric RAF dimer activation. *Biochemical Society Transactions*, **2014**, 42, 784-90	5.1	26
57	Anomalously Large Spectral Shifts near the Quantum Tunnelling Limit in Plasmonic Rulers with Subatomic Resolution. *Nano Letters*, **2019**, 19, 2051-2058	11.5	25
56	Controlling the structure and photophysics of fluorophore dimers using multiple cucurbit[8]uril clampings. *Chemical Science*, **2019**, 11, 812-825	9.4	25
55	Cucurbit[7]uril as a Supramolecular Artificial Enzyme for Diels Alder Reactions. *Angewandte Chemie* , **2017**, 129, 15894-15898	3.6	24
54	Coarse Master Equations for Binding Kinetics of Amyloid Peptide Dimers. *Journal of Physical Chemistry Letters*, **2016**, 7, 2676-82	6.4	24
53	Insights into functions of the H channel of cytochrome oxidase from atomistic molecular dynamics simulations. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E10339-E10348	11.5	24
52	Host-Guest Chemistry Meets Electrocatalysis: Cucurbit[6]uril on a Au Surface as a Hybrid System in CO Reduction. *ACS Catalysis*, **2020**, 10, 751-761	13.1	24
51	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, 2079-90	6.4	23
50	Mutations Decouple Proton Transfer from Phosphate Cleavage in the dUTPase Catalytic Reaction. *ACS Catalysis*, **2015**, 5, 3225-3237	13.1	22
49	On the Origins of the Linear Free Energy Relationships: Exploring the Nature of the Off-Diagonal Coupling Elements in S(N)2 Reactions. *Journal of Chemical Theory and Computation*, **2012**, 8, 3574-3585	6.4	22
48	Variational Identification of Markovian Transition States. *Physical Review X*, **2017**, 7,	9.1	21
47	Human DHEA sulfation requires direct interaction between PAPS synthase 2 and DHEA sulfotransferase SULT2A1. *Journal of Biological Chemistry*, **2018**, 293, 9724-9735	5.4	21
46	Structural Characterization of Arginine Fingers: Identification of an Arginine Finger for the Pyrophosphatase dUTPases. *Journal of the American Chemical Society*, **2016**, 138, 15035-15045	16.4	20
45	Cucurbit[8]uril-mediated pseudo[2,3]rotaxanes. *Chemical Communications*, **2019**, 55, 13227-13230	5.8	18
44	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, 6357-71	3.9	17
43	Turning Cucurbit[8]uril into a Supramolecular Nanoreactor for Asymmetric Catalysis. *Angewandte Chemie*, **2015**, 127, 13199-13203	3.6	17
42	Inhibiting Analyte Theft in Surface-Enhanced Raman Spectroscopy Substrates: Subnanomolar Quantitative Drug Detection. *ACS Sensors*, **2019**, 4, 2988-2996	9.2	15

41	Cations in motion: QM/MM studies of the dynamic and electrostatic roles of H and Mg ions in enzyme reactions. *Current Opinion in Structural Biology*, **2020**, 61, 198-206	8.1	15
40	Peptide dimerization-dissociation rates from replica exchange molecular dynamics. *Journal of Chemical Physics*, **2017**, 147, 152725	3.9	15
39	A Dynamic and Responsive Host in Action: Light-Controlled Molecular Encapsulation. *Angewandte Chemie*, **2016**, 128, 16330-16334	3.6	15
38	Calculating Kinetic Rates and Membrane Permeability from Biased Simulations. *Journal of Physical Chemistry B*, **2018**, 122, 11571-11578	3.4	15
37	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	13.1	14
36	Detecting mid-infrared light by molecular frequency upconversion in dual-wavelength nanoantennas. *Science*, **2021**, 374, 1268-1271	33.3	14
35	Smart supramolecular sensing with cucurbit[n]urils: probing hydrogen bonding with SERS. *Faraday Discussions*, **2017**, 205, 505-515	3.6	13
34	Modulating the oxidation of cucurbit[n]urils. *Organic and Biomolecular Chemistry*, **2017**, 15, 998-1005	3.9	12
33	Catalytic mechanism of 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, 10542-55	20.1	12
32	SARAH Domain-Mediated MST2-RASSF Dimeric Interactions. *PLoS Computational Biology*, **2016**, 12, e1005051	5	12
31	MST2-RASSF protein-protein interactions through SARAH domains. *Briefings in Bioinformatics*, **2016**, 17, 593-602	13.4	10
30	Mechanistic study of an immobilized molecular electrocatalyst by in situ gap-plasmon-assisted spectro-electrochemistry. *Nature Catalysis*, **2021**, 4, 157-163	36.5	10
29	Mean first passage times in variational coarse graining using Markov state models. *Journal of Chemical Physics*, **2019**, 150, 134107	3.9	9
28	Geometry and electronic structure of bis(tetrahydridoborato)bis(cyclopentadienyl)zirconium(IV). *Journal of Organometallic Chemistry*, **1999**, 582, 267-272	2.3	9
27	Optical probes of molecules as nano-mechanical switches. *Nature Communications*, **2020**, 11, 5905	17.4	9
26	Breaking the Selection Rules of Spin-Forbidden Molecular Absorption in Plasmonic Nanocavities. *ACS Photonics*, **2020**, 7, 2337-2342	6.3	9
25	Position-Dependent Diffusion from Biased Simulations and Markov State Model Analysis. *Journal of Chemical Theory and Computation*, **2021**, 17, 2022-2033	6.4	7
24	A simplified charge projection scheme for long-range electrostatics in ab initio QM/MM calculations. *Journal of Chemical Physics*, **2021**, 154, 024115	3.9	7

23	Correlation functions, mean first passage times, and the Kemeny constant. *Journal of Chemical Physics*, **2020**, 152, 104108	3.9	6
22	Limiting relaxation times from Markov state models. *Journal of Chemical Physics*, **2018**, 149, 072324	3.9	6
21	Representation of the QM Subsystem for Long-Range Electrostatic Interaction in Non-Periodic Ab Initio QM/MM Calculations. *Molecules*, **2018**, 23,	4.8	6
20	Divergence from the classical hydroboration reactivity; boron containing materials through a hydroboration cascade of small cyclic dienes. *Chemical Science*, **2015**, 6, 6262-6269	9.4	5
19	Direct Evidence for a Peroxide Intermediate and a Reactive Enzyme–Substrate–Dioxygen Configuration in a Cofactor-free Oxidase. *Angewandte Chemie*, **2014**, 126, 13930-13934	3.6	4
18	THE MIRROR SYSTEM HYPOTHESIS: FROM A MACAQUE-LIKE MIRROR SYSTEM TO IMITATION **2006**,		4
17	Organocatalytic Access to a -Cyclopentyl-amino Acid: An Intriguing Model of Selectivity and Formation of a Stable 10/12-Helix from the Corresponding Peptide. *Journal of the American Chemical Society*, **2020**, 142, 1382-1393	16.4	4
16	Efficient Irreversible Monte Carlo Samplers. *Journal of Chemical Theory and Computation*, **2020**, 16, 2124-2138	6.4	3
15	Spectroscopic Evidence for Peptide-Bond-Selective Ultraviolet Photodissociation. *Journal of Physical Chemistry Letters*, **2020**, 11, 206-209	6.4	3
14	Combining data integration and molecular dynamics for target identification in -Synuclein-aggregating neurodegenerative diseases: Structural insights on Synaptojanin-1 (Synj1). *Computational and Structural Biotechnology Journal*, **2020**, 18, 1032-1042	6.8	2
13	Deviation from the anti-Markovnikov rule: a computational study of the regio- and stereoselectivity of diene hydroboration reactions. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	2
12	Resolving sub-angstrom ambient motion through reconstruction from vibrational spectra. *Nature Communications*, **2021**, 12, 6759	17.4	2
11	The Dual Role of Histidine as General Base and Recruiter of a Third Metal Ion in HIV-1 RNase H		2
10	Toward Understanding CB[7]-Based Supramolecular Diels-Alder Catalysis. *Frontiers in Chemistry*, **2020**, 8, 587084	5	2
9	Gas-phase structures reflect the pain-relief potency of enkephalin peptides. *Physical Chemistry Chemical Physics*, **2019**, 21, 22700-22703	3.6	2
8	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	4.7	2
7	Nanoparticle surfactants for kinetically arrested photoactive assemblies to track light-induced electron transfer. *Nature Nanotechnology*, **2021**, 16, 1121-1129	28.7	2
6	The Role of Conserved Residues in the DEDDh Motif: the Proton-Transfer Mechanism of HIV-1 RNase H. *ACS Catalysis*, **2021**, 11, 7915-7927	13.1	1

5	Structural Dynamics and Catalytic Mechanism of ATP13A2 (PARK9) from Simulations. *Journal of Physical Chemistry B*, **2021**, 125, 11835-11847	3.4	0
4	Modelling the active SARS-CoV-2 helicase complex as a basis for structure-based inhibitor design. *Chemical Science*, **2021**, 12, 13492-13505	9.4	0
3	Simulated tempering with irreversible Gibbs sampling techniques. *Journal of Chemical Physics*, **2020** , 153, 214111	3.9	
2	Innentitelbild: A Dynamic and Responsive Host in Action: Light-Controlled Molecular Encapsulation (Angew. Chem. 52/2016). *Angewandte Chemie*, **2016**, 128, 16164-16164	3.6	
1	Phosphorylation of RAF Kinase Dimers Drives Conformational Changes that Facilitate Transactivation. *Angewandte Chemie*, **2016**, 128, 995-998	3.6	