

Mario Vazdar

List of Publications by Year in descending order

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74
papers

2,264
citations

218381

26
h-index

223531

46
g-index

77
all docs

77
docs citations

77
times ranked

3256
citing authors

#	ARTICLE	IF	CITATIONS
1	The on-the-fly surface-hopping program system Newton-X: Application to ab initio simulation of the nonadiabatic photodynamics of benchmark systems. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2007, 190, 228-240.	2.0	422
2	Arginine – Magic – Guanidinium Like-Charge Ion Pairing from Aqueous Salts to Cell Penetrating Peptides. <i>Accounts of Chemical Research</i> , 2018, 51, 1455-1464.	7.6	128
3	The nonadiabatic deactivation paths of pyrrole. <i>Journal of Chemical Physics</i> , 2006, 125, 164323.	1.2	101
4	Automerization reaction of cyclobutadiene and its barrier height: An ab initio benchmark multireference average-quadratic coupled cluster study. <i>Journal of Chemical Physics</i> , 2006, 125, 064310.	1.2	101
5	Ions at Hydrophobic Aqueous Interfaces: Molecular Dynamics with Effective Polarization. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2087-2091.	2.1	89
6	Polyarginine Interacts More Strongly and Cooperatively than Polylysine with Phospholipid Bilayers. <i>Journal of Physical Chemistry B</i> , 2016, 120, 9287-9296.	1.2	76
7	Excited-state non-adiabatic dynamics simulations of pyrrole. <i>Molecular Physics</i> , 2009, 107, 845-854.	0.8	65
8	Self-association of a highly charged arginine-rich cell-penetrating peptide. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 11428-11433.	3.3	63
9	Overcharging in Biological Systems: Reversal of Electrophoretic Mobility of Aqueous Polyaspartate by Multivalent Cations. <i>Physical Review Letters</i> , 2012, 108, 186101.	2.9	61
10	A surface-stabilized ozonide triggers bromide oxidation at the aqueous solution-vapour interface. <i>Nature Communications</i> , 2017, 8, 700.	5.8	59
11	Like-Charge Ion Pairing in Water: An Ab Initio Molecular Dynamics Study of Aqueous Guanidinium Cations. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2021-2024.	2.1	58
12	Cholesterol under oxidative stress – How lipid membranes sense oxidation as cholesterol is being replaced by oxysterols. <i>Free Radical Biology and Medicine</i> , 2015, 84, 30-41.	1.3	57
13	Mechanism of Long-Chain Free Fatty Acid Protonation at the Membrane-Water Interface. <i>Biophysical Journal</i> , 2018, 114, 2142-2151.	0.2	57
14	Like-Charge Guanidinium Pairing from Molecular Dynamics and Ab Initio Calculations. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11193-11201.	1.1	53
15	Orientational Dependence of the Affinity of Guanidinium Ions to the Water Surface. <i>Journal of Physical Chemistry B</i> , 2011, 115, 12521-12526.	1.2	44
16	Absorption and Fluorescence of PRODAN in Phospholipid Bilayers: A Combined Quantum Mechanics and Classical Molecular Dynamics Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 11428-11437.	1.1	43
17	The molecular mechanism behind reactive aldehyde action on transmembrane translocations of proton and potassium ions. <i>Free Radical Biology and Medicine</i> , 2015, 89, 1067-1076.	1.3	39
18	How cardiolipin peroxidation alters the properties of the inner mitochondrial membrane?. <i>Chemistry and Physics of Lipids</i> , 2018, 214, 15-23.	1.5	35

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19	Aggregation of Oligoarginines at Phospholipid Membranes: Molecular Dynamics Simulations, Time-Dependent Fluorescence Shift, and Biomimetic Colorimetric Assays. <i>Journal of Physical Chemistry B</i> , 2013, 117, 11530-11540.	1.2	34
20	Aqueous Guanidinium–Carbonate Interactions by Molecular Dynamics and Neutron Scattering: Relevance to Ion–Protein Interactions. <i>Journal of Physical Chemistry B</i> , 2013, 117, 1844-1848.	1.2	33
21	Behavior of 4-Hydroxynonenal in Phospholipid Membranes. <i>Journal of Physical Chemistry B</i> , 2012, 116, 6411-6415.	1.2	31
22	The study of hydrogen bonding and π - π interactions in phenol–ethynylbenzene complex by IR spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 132, 6-14.	2.0	31
23	Accurate Determination of the Orientational Distribution of a Fluorescent Molecule in a Phospholipid Membrane. <i>Journal of Physical Chemistry B</i> , 2014, 118, 855-863.	1.2	30
24	Matrix-controlled photofragmentation of formamide: dynamics simulation in argon by nonadiabatic QM/MM method. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 12719.	1.3	29
25	Metal-induced supramolecular chirality inversion of small self-assembled molecules in solution. <i>Chemical Communications</i> , 2017, 53, 1945-1948.	2.2	28
26	<i>Ab initio</i> quantum dynamical study of the multi-state nonadiabatic photodissociation of pyrrole. <i>Journal of Chemical Physics</i> , 2011, 135, 154310.	1.2	27
27	Electrodeposition of nano-sized nuclei of magnetic Co–Ni alloys onto n-Si (100). <i>Electrochemistry Communications</i> , 2001, 3, 159-163.	2.3	26
28	ANT1 Activation and Inhibition Patterns Support the Fatty Acid Cycling Mechanism for Proton Transport. <i>International Journal of Molecular Sciences</i> , 2021, 22, 2490.	1.8	25
29	Anomalous Protein–Protein Interactions in Multivalent Salt Solution. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3000-3006.	1.2	23
30	Mechanism of Cell Penetration by Permeabilization of Late Endosomes: Interplay between a Multivalent TAT Peptide and Bis(monoacylglycero)phosphate. <i>Cell Chemical Biology</i> , 2020, 27, 1296-1307.e5.	2.5	23
31	Guanidinium Pairing Facilitates Membrane Translocation. <i>Journal of Physical Chemistry B</i> , 2016, 120, 143-153.	1.2	22
32	Surface Propensity of Aqueous Atmospheric Bromine at the Liquid–Gas Interface. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3422-3429.	2.1	22
33	The effect of protonation on the photodissociation processes in formamide – An <i>ab initio</i> surface hopping dynamics study. <i>Chemical Physics</i> , 2008, 349, 308-318.	0.9	20
34	Reaction Mechanism of Covalent Modification of Phosphatidylethanolamine Lipids by Reactive Aldehydes 4-Hydroxy-2-nonenal and 4-Oxo-2-nonenal. <i>Chemical Research in Toxicology</i> , 2017, 30, 840-850.	1.7	19
35	Magnetic domain states in nano-sized Co nuclei electrodeposited onto monocrystalline silicon. <i>Materials Letters</i> , 2004, 58, 3518-3522.	1.3	17
36	Interactions of monovalent salts with cationic lipid bilayers. <i>Faraday Discussions</i> , 2013, 160, 341-358.	1.6	17

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37	Synthesis of Glycomimetics by Diastereoselective Passerini Reaction. <i>Journal of Organic Chemistry</i> , 2018, 83, 13146-13156.	1.7	17
38	Calculation of apparent pKa values of saturated fatty acids with different lengths in DOPC phospholipid bilayers. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10052-10060.	1.3	16
39	Mitochondrial Uncoupling Proteins (UCP1-UCP3) and Adenine Nucleotide Translocase (ANT1) Enhance the Protonophoric Action of 2,4-Dinitrophenol in Mitochondria and Planar Bilayer Membranes. <i>Biomolecules</i> , 2021, 11, 1178.	1.8	16
40	Synthesis of new 2-aminoimidazolones with antiproliferative activity via base promoted amino- β -lactam rearrangement. <i>Tetrahedron</i> , 2015, 71, 9202-9215.	1.0	14
41	Revisited Mechanism of Reaction between a Model Lysine Amino Acid Side Chain and 4-Hydroxynonenal in Different Solvent Environments. <i>Journal of Organic Chemistry</i> , 2019, 84, 526-535.	1.7	14
42	Ab Initio Study of the Reaction of Ozone with Bromide Ion. <i>Journal of Physical Chemistry A</i> , 2015, 119, 4482-4488.	1.1	13
43	Covalent modification of phosphatidylethanolamine by 4-hydroxy-2-nonenal increases sodium permeability across phospholipid bilayer membranes. <i>Free Radical Biology and Medicine</i> , 2019, 143, 433-440.	1.3	13
44	The Isomerization Barrier in Cyanocyclobutadienes: An ab Initio Multireference Average Quadratic Coupled Cluster Study. <i>Journal of Physical Chemistry A</i> , 2009, 113, 8351-8358.	1.1	11
45	Thermal reaction of [3,4]-benzo-8-substituted-3Z,5Z,7E-octatetraenes and quantum-chemical study of the β -electrocyclisation. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 6771.	1.5	11
46	QM/MM non-adiabatic decay dynamics of formamide in polar and non-polar solvents. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 13262.	1.3	11
47	Molecular Dynamics Simulations of the Elusive Matrix-Open State of Mitochondrial ADP/ATP Carrier. <i>Israel Journal of Chemistry</i> , 2020, 60, 735-743.	1.0	11
48	Photocyclization of Tetra- and Pentapeptides Containing Adamantylphthalimide and Phenylalanines: Reaction Efficiency and Diastereoselectivity. <i>Journal of Organic Chemistry</i> , 2018, 83, 14905-14922.	1.7	10
49	Anomalous surface behavior of hydrated guanidinium ions due to ion pairing. <i>Journal of Chemical Physics</i> , 2018, 148, 144508.	1.2	10
50	Zwitterionic structures of strained cis-pyramidalized disilenes: fact or artifact. <i>Theoretical Chemistry Accounts</i> , 2009, 124, 421-430.	0.5	8
51	Desaturase specificity is controlled by the physicochemical properties of a single amino acid residue in the substrate binding tunnel. <i>Computational and Structural Biotechnology Journal</i> , 2020, 18, 1202-1209.	1.9	8
52	Molecular Dynamics Simulations of Mitochondrial Uncoupling Protein 2. <i>International Journal of Molecular Sciences</i> , 2021, 22, 1214.	1.8	8
53	Formamide as the Model Compound for Photodissociation Studies of the Peptide Bond. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2010, , 77-106.	0.6	7
54	Does fluoride disrupt hydrogen bond network in cationic lipid bilayer? Time-dependent fluorescence shift of Laurdan and molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2014, 141, 22D516.	1.2	6

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55	High pressure promoted exchange of guests from hemicarceplexes. <i>Tetrahedron</i> , 2015, 71, 550-553.	1.0	6
56	Computation and volumetric insight into (p,T) effect on aqueous guanidinium chloride. <i>Journal of Chemical Thermodynamics</i> , 2021, 158, 106450.	1.0	5
57	Acetamide as the model of the peptide bond: Nonadiabatic photodynamical simulations in the gas phase and in the argon matrix. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 136-143.	1.1	4
58	The Antiferromagnetic Spin Coupling in Nonâ€KekulÃ© Acenesâ€”Impressive Polyradical Character Revealed by Highâ€Level Multireference Methods. <i>ChemPhysChem</i> , 2016, 17, 2013-2021.	1.0	4
59	Unraveling the weak hydrogen bonds of ethynylpyridines and ethynylbenzene with trimethylphosphate â€” A combined FT-Raman spectroscopic and quantum-chemical study. <i>Journal of Molecular Liquids</i> , 2016, 218, 499-507.	2.3	4
60	Temperature-induced release of crystal water in the Co, Mo and Pt complexes of N,N-diacetatedithiocarbamate. FTIR spectroscopy and quantum chemical study. <i>Journal of Molecular Structure</i> , 2016, 1103, 245-253.	1.8	4
61	Coarse-grained model of titrating peptides interacting with lipid bilayers. <i>Journal of Chemical Physics</i> , 2018, 149, 244108.	1.2	4
62	Model Systems for Dynamics of Î€-Conjugated Biomolecules in Excited States. , 2012, , 1175-1213.		3
63	The exploration of hydrogen bonding properties of 2,6- and 3,5-diethynylpyridine by IR spectroscopy. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 1912-1923.	2.0	3
64	Distributions of therapeutically promising neurosteroids in cellular membranes. <i>Chemistry and Physics of Lipids</i> , 2017, 203, 78-86.	1.5	3
65	Vibrational spectroscopy combined with molecular dynamics simulations as a tool for studying behavior of reactive aldehydes inserted in phospholipid bilayers. <i>Chemistry and Physics of Lipids</i> , 2019, 225, 104793.	1.5	3
66	Chemistry and Reactivity of 4-hydroxy-2-nonenal (HNE) in Model Biological Systems. <i>Mini-Reviews in Medicinal Chemistry</i> , 2021, 21, 1394-1405.	1.1	3
67	A computational study of regioselectivity in Î²-lactam iminothiazolidinone formation. <i>Tetrahedron Letters</i> , 2015, 56, 6908-6911.	0.7	2
68	Model Systems for Dynamics of Î€-Conjugated Biomolecules in Excited States. , 2017, , 1697-1739.		1
69	Membrane Lipids Alter Uncoupling Effect of 2,4 Dinitrophenol. <i>Biophysical Journal</i> , 2019, 116, 511a.	0.2	0
70	A Computational Insight into Reaction Between Different Amino Acids with Reactive Aldehydes 4-hydroxy-2-nonenal and 4-oxo-2-nonenal. <i>Croatica Chemica Acta</i> , 2019, 92, 229-239.	0.1	0
71	Molecular dynamics study of functionally relevant interdomain and active site interactions in the autotransporter esterase EstA from <i>Pseudomonas aeruginosa</i> . <i>Molecular Simulation</i> , 2020, 46, 743-756.	0.9	0
72	Multireference Configuration Interaction Methods â€” An Application to the Valence Isomerism in Cyclobutadieno-p-benzoquinone and its Diprotonated Form. <i>Croatica Chemica Acta</i> , 2015, 88, 495-503.	0.1	0

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73	Model Systems for Dynamics of I^{E} -Conjugated Biomolecules in Excited States. , 2016, , 1-43.		0
74	Mechanism of Cell Penetration by Permeabilization of Late Endosomes: Interplay between a Multivalent TAT-Like Cell-Penetrating Peptide and the Lipid Bis(Monoacylglycerol)Phosphate. SSRN Electronic Journal, 0, , .	0.4	0