

Dorit Shemesh

List of Publications by Year in descending order

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29
papers

746
citations

471509

17
h-index

552781

26
g-index

30
all docs

30
docs citations

30
times ranked

787
citing authors

#	ARTICLE	IF	CITATIONS
1	Computational Studies of Atmospherically-Relevant Chemical Reactions in Water Clusters and on Liquid Water and Ice Surfaces. <i>Accounts of Chemical Research</i> , 2015, 48, 399-406.	15.6	89
2	Efficient Excited-State Deactivation of the Gly-Phe-Ala Tripeptide via an Electron-Driven Proton-Transfer Process. <i>Journal of the American Chemical Society</i> , 2009, 131, 1374-1375.	13.7	65
3	Experimental and Theoretical Study of Aqueous <i>cis</i> -Pinonic Acid Photolysis. <i>Journal of Physical Chemistry A</i> , 2013, 117, 12930-12945.	2.5	60
4	Computational Studies of the Photophysics of Neutral and Zwitterionic Amino Acids in an Aqueous Environment: Tyrosine $\hat{\sim}$ (H ₂ O) ₂ and Tryptophan $\hat{\sim}$ (H ₂ O) ₂ Clusters. <i>Journal of Physical Chemistry A</i> , 2009, 113, 542-550.	2.5	57
5	Absorption Spectra and Photolysis of Methyl Peroxide in Liquid and Frozen Water. <i>Journal of Physical Chemistry A</i> , 2012, 116, 6068-6077.	2.5	49
6	Photochemistry of Thin Solid Films of the Neonicotinoid Imidacloprid on Surfaces. <i>Environmental Science & Technology</i> , 2017, 51, 2660-2668.	10.0	37
7	Ab initio and semi-empirical Molecular Dynamics simulations of chemical reactions in isolated molecules and in clusters. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 9760-9775.	2.8	35
8	Role of excited-state hydrogen detachment and hydrogen-transfer processes for the excited-state deactivation of an aromatic dipeptide: N-acetyl tryptophan methyl amide. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 4899.	2.8	29
9	Photophysics of the Trp-Gly dipeptide: Role of electron and proton transfer processes for efficient excited-state deactivation. <i>Chemical Physics Letters</i> , 2009, 482, 38-43.	2.6	27
10	Vibrational spectroscopy for glycine adsorbed on silicon clusters: Harmonic and anharmonic calculations for models of the Si(100)-2 $\hat{\text{A}}$ -1 surface. <i>Chemical Physics</i> , 2008, 347, 218-228.	1.9	26
11	Dynamics of Triplet-State Photochemistry of Pentanal: Mechanisms of Norrish I, Norrish II, and H Abstraction Reactions. <i>Journal of Physical Chemistry A</i> , 2013, 117, 11711-11724.	2.5	26
12	Different chemical dynamics for different conformers of biological molecules: Photoionization of glycine. <i>Journal of Chemical Physics</i> , 2005, 122, 241104.	3.0	24
13	Photoionization Dynamics of Glycine: The First 10 Picoseconds. <i>Journal of Physical Chemistry A</i> , 2004, 108, 11477-11484.	2.5	22
14	Absorption spectra and aqueous photochemistry of $\hat{\text{I}}^2$ -hydroxyalkyl nitrates of atmospheric interest. <i>Molecular Physics</i> , 2015, 113, 2179-2190.	1.7	22
15	Femtosecond timescale deactivation of electronically excited peroxides at ice surfaces. <i>Molecular Physics</i> , 2012, 110, 605-617.	1.7	21
16	Photochemistry of aldehyde clusters: cross-molecular versus unimolecular reaction dynamics. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 23861-23868.	2.8	21
17	Absorption spectra of pyruvic acid in water: insights from calculations for small hydrates and comparison to experiment. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 12658-12670.	2.8	19
18	Classical Trajectory Simulations of Photoionization Dynamics of Tryptophan: Intramolecular Energy Flow, Hydrogen-Transfer Processes and Conformational Transitions. <i>Journal of Physical Chemistry A</i> , 2006, 110, 8401-8408.	2.5	18

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19	Impact of pH and NaCl and CaCl ₂ Salts on the Speciation and Photochemistry of Pyruvic Acid in the Aqueous Phase. <i>Journal of Physical Chemistry A</i> , 2020, 124, 5071-5080.	2.5	18
20	Photochemical Reactions of Cyclohexanone: Mechanisms and Dynamics. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7112-7120.	2.5	17
21	Photoionization dynamics of glycine adsorbed on a silicon cluster: "On-the-fly" simulations. <i>Journal of Chemical Physics</i> , 2005, 122, 184704.	3.0	15
22	Molecular Dynamics of Photoinduced Reactions of Acrylic Acid: Products, Mechanisms, and Comparison with Experiment. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 527-533.	4.6	15
23	Effect of the Chirality of Residues and Turns on the Electronic Excitation Spectra, Excited-State Reaction Paths and Conical Intersections of Capped Phenylalanine-Alanine Dipeptides. <i>ChemPhysChem</i> , 2011, 12, 1833-1840.	2.1	14
24	DMAP-assisted sulfonylation as an efficient step for the methylation of primary amine motifs on solid support. <i>Beilstein Journal of Organic Chemistry</i> , 2017, 13, 806-816.	2.2	9
25	Experimental and Theoretical Studies of the Environmental Sensitivity of the Absorption Spectra and Photochemistry of Nitenpyram and Analogs. <i>ACS Earth and Space Chemistry</i> , 2019, 3, 2063-2075.	2.7	8
26	Adjacent keto and enol groups in photochemistry of a cyclic molecule: Products, mechanisms and dynamics. <i>Chemical Physics</i> , 2018, 515, 177-186.	1.9	3
27	Dynamical Simulations of Photoionization of Small Biological Molecules. , 2006, , 213-237.		0
28	Dynamics of Photochemical Reactions of Organic Carbonyls and their Clusters. <i>Advances in Chemical Physics</i> , 2016, , 1-22.	0.3	0
29	Photophysics of the Trp-Gly Dipeptide: Role of Electron and Proton Transfer Processes for Efficient Excited-State Deactivation. , 2010, , 641-649.		0