

Tolga N V Karsili

List of Publications by Year in descending order

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65
papers

1,421
citations

331259

21
h-index

344852

36
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65
all docs

65
docs citations

65
times ranked

1614
citing authors

#	ARTICLE	IF	CITATIONS
1	Photoprotection: extending lessons learned from studying natural sunscreens to the design of artificial sunscreen constituents. <i>Chemical Society Reviews</i> , 2017, 46, 3770-3791.	18.7	146
2	Probing the Ultrafast Energy Dissipation Mechanism of the Sunscreen Oxybenzone after UVA Irradiation. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 1363-1368.	2.1	97
3	<i>Ab Initio</i> Study of Potential Ultrafast Internal Conversion Routes in Oxybenzone, Caffeic Acid, and Ferulic Acid: Implications for Sunscreens. <i>Journal of Physical Chemistry A</i> , 2014, 118, 11999-12010.	1.1	90
4	Mechanism of Photocatalytic Water Splitting with Graphitic Carbon Nitride: Photochemistry of the Heptazine-Water Complex. <i>Journal of Physical Chemistry A</i> , 2017, 121, 4754-4764.	1.1	85
5	A "bottom up" <i>ab initio</i> computational approach to understanding fundamental photophysical processes in nitrogen containing heterocycles, DNA bases and base pairs. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20007-20027.	1.3	78
6	Exploring quantum phenomena and vibrational control in $\tilde{I}f^*$ mediated photochemistry. <i>Chemical Science</i> , 2013, 4, 993-1001.	3.7	67
7	O-H bond fission in 4-substituted phenols: S1 state predissociation viewed in a Hammett-like framework. <i>Chemical Science</i> , 2013, 4, 2434.	3.7	46
8	Solvent induced conformer specific photochemistry of guaiacol. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 16187.	1.3	41
9	Photocatalytic Water Splitting with the Acridine Chromophore: A Computational Study. <i>Journal of Physical Chemistry B</i> , 2015, 119, 10664-10672.	1.2	41
10	Symmetry matters: photodissociation dynamics of symmetrically versus asymmetrically substituted phenols. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 588-598.	1.3	38
11	Theoretical insights into the photo-protective mechanisms of natural biological sunscreens: building blocks of eumelanin and pheomelanin. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 3644-3658.	1.3	34
12	Photoinduced water splitting via benzoquinone and semiquinone sensitisation. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 32183-32193.	1.3	30
13	Toolbox of Nonmetallocene Lanthanides: Multifunctional Catalysts in Group-Transfer Polymerization. <i>Inorganic Chemistry</i> , 2017, 56, 9754-9764.	1.9	30
14	Comparative study of methodologies for calculating metastable states of small to medium-sized molecules. <i>Journal of Chemical Physics</i> , 2019, 151, 244104.	1.2	30
15	Exploring the Dynamics of the Photoinduced Ring-Opening of Heterocyclic Molecules. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3440-3451.	2.1	28
16	Competing $\tilde{I}\tilde{e}f^*$ mediated dynamics in mequinol: O-H versus O-CH3 photodissociation pathways. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 13415.	1.3	27
17	UV Photodissociation of Pyrroles: Symmetry and Substituent Effects. <i>Journal of Physical Chemistry A</i> , 2013, 117, 12067-12074.	1.1	26
18	Dynamics of the A-band ultraviolet photodissociation of methyl iodide and ethyl iodide via velocity-map imaging with "universal" detection. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 4096-4106.	1.3	26

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19	Exploring Norrish type I and type II reactions: an <i>ab initio</i> mechanistic study highlighting singlet-state mediated chemistry. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 14418-14428.	1.3	24
20	Towards Understanding Photodegradation Pathways in Lignins: The Role of Intramolecular Hydrogen Bonding in Excited States. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 2138-2143.	2.1	22
21	Ultrafast Excited-State Dynamics of 2,4-Dimethylpyrrole. <i>Journal of Physical Chemistry A</i> , 2014, 118, 10909-10918.	1.1	21
22	Photofragmentation Dynamics in Solution Probed by Transient IR Absorption Spectroscopy: $\tilde{\text{I}}\tilde{\text{C}}\tilde{\text{I}}\tilde{\text{f}}^*$ -Mediated Bond Cleavage in <i>p</i> -Methylthiophenol and <i>p</i> -Methylthioanisole. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 3715-3720.	2.1	20
23	First Step toward a Universal Fluorescent Probe: Unravelling the Photodynamics of an Amino Maleimide Fluorophore. <i>Journal of Physical Chemistry A</i> , 2017, 121, 6357-6365.	1.1	20
24	MOF-based electrocatalysts for high-efficiency CO_2 conversion: structure, performance, and perspectives. <i>Journal of Materials Chemistry A</i> , 2021, 9, 22710-22728.	5.2	20
25	Excited-State Deactivation of Adenine by Electron-Driven Proton Transfer Reactions in Adenine Water Clusters: A Computational Study. <i>ChemPhysChem</i> , 2016, 17, 1298-1304.	1.0	19
26	An exploration of the reactivity of singlet oxygen with biomolecular constituents. <i>Chemical Communications</i> , 2016, 52, 10996-10999.	2.2	18
27	Photodissociation dynamics of the pyridinyl radical: Time-dependent quantum wave-packet calculations. <i>Journal of Chemical Physics</i> , 2017, 146, 124304.	1.2	18
28	A Simple and Efficient Method for Simulating the Electronic Absorption Spectra of Criegee Intermediates: Benchmarking on CH_2OO and CH_3CHOO . <i>Journal of Physical Chemistry A</i> , 2021, 125, 4089-4097.	1.1	18
29	Near ultraviolet photochemistry of 2-bromo- and 2-iodothiophene: Revealing photoinduced ring opening in the gas phase?. <i>Journal of Chemical Physics</i> , 2015, 142, 224303.	1.2	17
30	Photodissociation Dynamics of CH_2OO on Multiple Potential Energy Surfaces: Experiment and Theory. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6571-6579.	1.1	16
31	Fragmentation dynamics of the ethyl bromide and ethyl iodide cations: a velocity-map imaging study. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 2167-2178.	1.3	15
32	Tuning photochemistry: substituent effects on $\tilde{\text{I}}\tilde{\text{C}}\tilde{\text{I}}\tilde{\text{f}}^*$ state mediated bond fission in thioanisoles. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 16246-16256.	1.3	14
33	The near ultraviolet photodissociation dynamics of 2- and 3-substituted thiophenols: Geometric vs. electronic structure effects. <i>Journal of Chemical Physics</i> , 2017, 147, 013923.	1.2	14
34	Photoinduced C-H bond fission in prototypical organic molecules and radicals. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 13880-13901.	1.3	14
35	Photodissociation dynamics of methyl vinyl ketone oxide: A four-carbon unsaturated Criegee intermediate from isoprene ozonolysis. <i>Journal of Chemical Physics</i> , 2021, 155, 174305.	1.2	14
36	Insights into the Ultrafast Dynamics of CH_2OO and CH_3CHOO Following Excitation to the Bright $\tilde{\text{I}}\tilde{\text{C}}\tilde{\text{I}}\tilde{\text{f}}^*$ State: The Role of Singlet and Triplet States. <i>Photochemistry and Photobiology</i> , 2021, , .	1.3	12

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37	Mechanisms of H and CO loss from the uracil nucleobase following low energy electron irradiation. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17233-17241.	1.3	11
38	Role of Electron-Driven Proton-Transfer Processes in the Ultrafast Deactivation of Photoexcited Anionic 8-oxoGuanine-Adenine and 8-oxoGuanine-Cytosine Base Pairs. <i>Molecules</i> , 2017, 22, 135.	1.7	11
39	Electronic Absorption Spectroscopy and Photochemistry of Criegee Intermediates. <i>Photochemistry and Photobiology</i> , 2023, 99, 4-18.	1.3	11
40	Mechanistic insights into excited state intramolecular proton transfer in isolated and metal chelated supramolecular chemosensors. <i>Dalton Transactions</i> , 2016, 45, 18921-18930.	1.6	10
41	Mechanistic insights into photoinduced damage of DNA and RNA nucleobases in the gas phase and in bulk solution. <i>Faraday Discussions</i> , 2018, 207, 329-350.	1.6	10
42	Modeling the Conformer-Dependent Electronic Absorption Spectra and Photolysis Rates of Methyl Vinyl Ketone Oxide and Methacrolein Oxide. <i>Journal of Physical Chemistry A</i> , 2022, 126, 485-496.	1.1	10
43	Photofragmentation dynamics of N,N-dimethylformamide following excitation at 193 nm. <i>Journal of Chemical Physics</i> , 2017, 147, 013941.	1.2	9
44	Mechanisms of photoreactivity in hydrogen-bonded adenine-H ₂ O complexes. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 14238-14249.	1.3	9
45	Extreme population inversion in the fragments formed by UV photoinduced S-H bond fission in 2-thiophenethiol. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 11401-11410.	1.3	8
46	Structure, DFT Calculations, and Magnetic Characterization of Coordination Polymers of Bridged Dicyanamido-Metal(II) Complexes. <i>Magnetochemistry</i> , 2019, 5, 41.	1.0	6
47	Photocrosslinking between nucleic acids and proteins: general discussion. <i>Faraday Discussions</i> , 2018, 207, 283-306.	1.6	5
48	Origins of Photodamage in Pheomelanin Constituents: Photochemistry of 4-Hydroxybenzothiazole. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1986-1993.	1.1	5
49	Steric Effects of Alkyl Substituents at N-Donor Bidentate Amines Direct the Nuclearity, Bonding and Bridging Modes in Isothiocyanato-Copper(II) Coordination Compounds. <i>Crystals</i> , 2019, 9, 38.	1.0	5
50	Affordable Setup for Studying Photochemistry in Action in Undergraduate Teaching Laboratories: Principles and Applications. <i>Journal of Chemical Education</i> , 2020, 97, 2203-2211.	1.1	5
51	Photofragment Translational Spectroscopy Studies of H Atom Loss Following Ultraviolet Photoexcitation of Methimazole in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2018, 122, 9869-9878.	1.1	4
52	Hydrogen-Deuterium Exchange in Basic Near-Critical and Supercritical Media: An Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2020, 124, 2530-2536.	1.1	4
53	Electron-induced origins of prebiotic building blocks of sugars: mechanism of self-reactions of a methanol anion dimer. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 12599-12607.	1.3	3
54	The role of 1 ^π σ* states in the formation of adenine radical-cations in DNA duplexes. <i>Chemical Physics</i> , 2018, 515, 464-471.	0.9	3

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55	Quantifying rival bond fission probabilities following photoexcitation: C–S bond fission in <i>n</i> -butylmethylsulfide. <i>Chemical Science</i> , 2019, 10, 5290-5298.	3.7	3
56	The Role of Norrish Type-I Chemistry in Photoactive Drugs: An ab initio Study of a Cyclopropanone-Enediyne Drug Precursor. <i>Frontiers in Chemistry</i> , 2020, 8, 596590.	1.8	3
57	The states that hide in the shadows: the potential role of conical intersections in the ground state unimolecular decay of a Criegee intermediate. <i>Physical Chemistry Chemical Physics</i> , 2021, 24, 532-540.	1.3	3
58	Role of Pr-Vacancies and O-Interstitials on the Activity and Stability of (Pr _{1-x} Ln _x) ₂ NiO ₄ (Ln = La, Nd, Pm, Sm, Gd, Tb, Dy, and Tm) Oxides. <i>Journal of Physical Chemistry C</i> , 2021, 125, 124508.	1.3	3
59	Oxidative Addition of Singlet Oxygen to Model Building Blocks of the Aerucyclamide A Peptide: A First-Principles Approach. <i>Journal of Physical Chemistry A</i> , 2020, 124, 498-504.	1.1	2
60	Light induced charge and energy transport in nucleic acids and proteins: general discussion. <i>Faraday Discussions</i> , 2018, 207, 153-180.	1.6	1
61	Ultraviolet photodissociation of gas-phase transition metal complexes: dicarbonylcyclopentadienyliodoiron(II). <i>Molecular Physics</i> , 2021, 119, e1813343.	0.8	1
62	Light induced damage and repair in nucleic acids and proteins: general discussion. <i>Faraday Discussions</i> , 2018, 207, 389-408.	1.6	0
63	Bionanophotonics: general discussion. <i>Faraday Discussions</i> , 2018, 207, 491-512.	1.6	0
64	Photoprotective Properties of Eumelanin: Computational Insights into the Photophysics of a Catechol:Quinone Heterodimer Model System. <i>Photochem</i> , 2021, 1, 26-37.	1.3	0
65	Simulating Electronic Absorption Spectra of Atmospherically Relevant Molecules: A Systematic Assignment for Enhancing Undergraduate STEM Education. <i>Education Sciences</i> , 2022, 12, 252.	1.4	0