Tolga N V Karsili

List of Publications by Year
in descending order

65	1,421	331259	344852
papers	citations	21 h-index	36 g-index

65	65	65	1614
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Electronic Absorption Spectroscopy and Photochemistry of Criegee Intermediates. Photochemistry and Photobiology, 2023, 99, 4-18.	1.3	11
2	Modeling the Conformer-Dependent Electronic Absorption Spectra and Photolysis Rates of Methyl Vinyl Ketone Oxide and Methacrolein Oxide. Journal of Physical Chemistry A, 2022, 126, 485-496.	1.1	10
3	Simulating Electronic Absorption Spectra of Atmospherically Relevant Molecules: A Systematic Assignment for Enhancing Undergraduate STEM Education. Education Sciences, 2022, 12, 252.	1.4	0
4	Ultraviolet photodissociation of gas-phase transition metal complexes: dicarbonylcyclopentadienyliodoiron(II). Molecular Physics, 2021, 119, e1813343.	0.8	1
5	MOF-based electrocatalysts for high-efficiency CO₂ conversion: structure, performance, and perspectives. Journal of Materials Chemistry A, 2021, 9, 22710-22728.	5.2	20
6	Photoprotective Properties of Eumelanin: Computational Insights into the Photophysics of a Catechol:Quinone Heterodimer Model System. Photochem, 2021, 1, 26-37.	1.3	0
7	A Simple and Efficient Method for Simulating the Electronic Absorption Spectra of Criegee Intermediates: Benchmarking on CH₂OO and CH₃CHOO. Journal of Physical Chemistry A, 2021, 125, 4089-4097.	1.1	18
8	Photodissociation Dynamics of CH₂OO on Multiple Potential Energy Surfaces: Experiment and Theory. Journal of Physical Chemistry A, 2021, 125, 6571-6579.	1.1	16
9	Photodissociation dynamics of methyl vinyl ketone oxide: A four-carbon unsaturated Criegee intermediate from isoprene ozonolysis. Journal of Chemical Physics, 2021, 155, 174305.	1.2	14
10	Insights into the Ultrafast Dynamics of CH 2 OO and CH 3 CHOO Following Excitation to the Bright 1 Ï€Ï€* State: The Role of Singlet and Triplet States. Photochemistry and Photobiology, 2021, , .	1.3	12
11	The states that hide in the shadows: the potential role of conical intersections in the ground state unimolecular decay of a Criegee intermediate. Physical Chemistry Chemical Physics, 2021, 24, 532-540.	1.3	3
12	Role of Pr-Vacancies and O-Interstitials on the Activity and Stability of (Pr_{1â^'x}Ln_x)₂NiO₄ (Ln = La, Nd, Pm, Sm, Gd, Tb, Dy, and) Tj ETQq0 0 0 rgBT /Overlo 168, 124508.	1.3	3
13	Oxidative Addition of Singlet Oxygen to Model Building Blocks of the Aerucyclamide A Peptide: A First-Principles Approach. Journal of Physical Chemistry A, 2020, 124, 498-504.	1.1	2
14	Affordable Setup for Studying Photochemistry in Action in Undergraduate Teaching Laboratories: Principles and Applications. Journal of Chemical Education, 2020, 97, 2203-2211.	1.1	5
15	The Role of Norrish Type-I Chemistry in Photoactive Drugs: An ab initio Study of a Cyclopropenone-Enediyne Drug Precursor. Frontiers in Chemistry, 2020, 8, 596590.	1.8	3
16	Hydrogenâ€“Deuterium Exchange in Basic Near-Critical and Supercritical Media: An Experimental and Theoretical Study. Journal of Physical Chemistry A, 2020, 124, 2530-2536.	1.1	4
17	Structure, DFT Calculations, and Magnetic Characterization of Coordination Polymers of Bridged Dicyanamido-Metal(II) Complexes. Magnetochemistry, 2019, 5, 41.	1.0	6
18	Steric Effects of Alkyl Substituents at N-Donor Bidentate Amines Direct the Nuclearity, Bonding and Bridging Modes in Isothiocyanato-Copper(II) Coordination Compounds. Crystals, 2019, 9, 38.	1.0	5

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19	Mechanisms of photoreactivity in hydrogen-bonded adenineâ€“H₂O complexes. Physical Chemistry Chemical Physics, 2019, 21, 14238-14249.	1.3	9
20	Photoinduced Câ€“H bond fission in prototypical organic molecules and radicals. Physical Chemistry Chemical Physics, 2019, 21, 13880-13901.	1.3	14
21	Quantifying rival bond fission probabilities following photoexcitation: Câ€“S bond fission in t-butylmethylsulfide. Chemical Science, 2019, 10, 5290-5298.	3.7	3
22	Exploring Norrish type I and type II reactions: an ab initio mechanistic study highlighting singlet-state mediated chemistry. Physical Chemistry Chemical Physics, 2019, 21, 14418-14428.	1.3	24
23	Comparative study of methodologies for calculating metastable states of small to medium-sized molecules. Journal of Chemical Physics, 2019, 151, 244104.	1.2	30
24	Electron-induced origins of prebiotic building blocks of sugars: mechanism of self-reactions of a methanol anion dimer. Physical Chemistry Chemical Physics, 2018, 20, 12599-12607.	1.3	3
25	Light induced damage and repair in nucleic acids and proteins: general discussion. Faraday Discussions, 2018, 207, 389-408.	1.6	0
26	Photocrosslinking between nucleic acids and proteins: general discussion. Faraday Discussions, 2018, 207, 283-306.	1.6	5
27	Light induced charge and energy transport in nucleic acids and proteins: general discussion. Faraday Discussions, 2018, 207, 153-180.	1.6	1
28	Bionanophotonics: general discussion. Faraday Discussions, 2018, 207, 491-512.	1.6	0
29	Origins of Photodamage in Pheomelanin Constituents: Photochemistry of 4-Hydroxybenzothiazole. Journal of Physical Chemistry A, 2018, 122, 1986-1993.	1.1	5
30	Mechanistic insights into photoinduced damage of DNA and RNA nucleobases in the gas phase and in bulk solution. Faraday Discussions, 2018, 207, 329-350.	1.6	10
31	Photofragment Translational Spectroscopy Studies of H Atom Loss Following Ultraviolet Photoexcitation of Methimazole in the Gas Phase. Journal of Physical Chemistry A, 2018, 122, 9869-9878.	1.1	4
32	The role of 1Ï€Ïƒâˆ— states in the formation of adenine radical-cations in DNA duplexes. Chemical Physics, 2018, 515, 464-471.	0.9	3
33	Mechanisms of H and CO loss from the uracil nucleobase following low energy electron irradiation. Physical Chemistry Chemical Physics, 2017, 19, 17233-17241.	1.3	11
34	Mechanism of Photocatalytic Water Splitting with Graphitic Carbon Nitride: Photochemistry of the Heptazineâ€“Water Complex. Journal of Physical Chemistry A, 2017, 121, 4754-4764.	1.1	85
35	Photofragmentation dynamics of N,N-dimethylformamide following excitation at 193 nm. Journal of Chemical Physics, 2017, 147, 013941.	1.2	9
36	The near ultraviolet photodissociation dynamics of 2- and 3-substituted thiophenols: Geometric vs. electronic structure effects. Journal of Chemical Physics, 2017, 147, 013923.	1.2	14

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37	Photodissociation dynamics of the pyridinyl radical: Time-dependent quantum wave-packet calculations. Journal of Chemical Physics, 2017, 146, 124304.	1.2	18
38	Toolbox of Nonmetallocene Lanthanides: Multifunctional Catalysts in Group-Transfer Polymerization. Inorganic Chemistry, 2017, 56, 9754-9764.	1.9	30
39	First Step toward a Universal Fluorescent Probe: Unravelling the Photodynamics of an Aminoâ€“Maleimide Fluorophore. Journal of Physical Chemistry A, 2017, 121, 6357-6365.	1.1	20
40	Exploring the Dynamics of the Photoinduced Ring-Opening of Heterocyclic Molecules. Journal of Physical Chemistry Letters, 2017, 8, 3440-3451.	2.1	28
41	Role of Electron-Driven Proton-Transfer Processes in the Ultrafast Deactivation of Photoexcited Anionic 8-oxoGuanine-Adenine and 8-oxoGuanine-Cytosine Base Pairs. Molecules, 2017, 22, 135.	1.7	11
42	Photoprotection: extending lessons learned from studying natural sunscreens to the design of artificial sunscreen constituents. Chemical Society Reviews, 2017, 46, 3770-3791.	18.7	146
43	Extreme population inversion in the fragments formed by UV photoinduced Sâ€“H bond fission in 2-thiophenethiol. Physical Chemistry Chemical Physics, 2016, 18, 11401-11410.	1.3	8
44	An exploration of the reactivity of singlet oxygen with biomolecular constituents. Chemical Communications, 2016, 52, 10996-10999.	2.2	18
45	Mechanistic insights into excited state intramolecular proton transfer in isolated and metal chelated supramolecular chemosensors. Dalton Transactions, 2016, 45, 18921-18930.	1.6	10
46	Excitedâ€State Deactivation of Adenine by Electronâ€Driven Protonâ€Transfer Reactions in Adenineâ€“Water Clusters: Aâ€…Computational Study. ChemPhysChem, 2016, 17, 1298-1304.	1.0	19
47	A â€˜bottom upâ€™, ab initio computational approach to understanding fundamental photophysical processes in nitrogen containing heterocycles, DNA bases and base pairs. Physical Chemistry Chemical Physics, 2016, 18, 20007-20027.	1.3	78
48	Theoretical insights into the photo-protective mechanisms of natural biological sunscreens: building blocks of eumelanin and pheomelanin. Physical Chemistry Chemical Physics, 2016, 18, 3644-3658.	1.3	34
49	Tuning photochemistry: substituent effects on ΪϵΪƒ* state mediated bond fission in thioanisoles. Physical Chemistry Chemical Physics, 2015, 17, 16246-16256.	1.3	14
50	Dynamics of the A-band ultraviolet photodissociation of methyl iodide and ethyl iodide via velocity-map imaging with â€˜universalâ€™ detection. Physical Chemistry Chemical Physics, 2015, 17, 4096-4106.	1.3	26
51	Probing the Ultrafast Energy Dissipation Mechanism of the Sunscreen Oxybenzone after UVA Irradiation. Journal of Physical Chemistry Letters, 2015, 6, 1363-1368.	2.1	97
52	Photocatalytic Water Splitting with the Acridine Chromophore: A Computational Study. Journal of Physical Chemistry B, 2015, 119, 10664-10672.	1.2	41
53	Near ultraviolet photochemistry of 2-bromo- and 2-iodothiophene: Revealing photoinduced ring opening in the gas phase?. Journal of Chemical Physics, 2015, 142, 224303.	1.2	17
54	Photoinduced water splitting via benzoquinone and semiquinone sensitisation. Physical Chemistry Chemical Physics, 2015, 17, 32183-32193.	1.3	30

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55	Ultrafast Excited-State Dynamics of 2,4-Dimethylpyrrole. Journal of Physical Chemistry A, 2014, 118, 10909-10918.	1.1	21
56	Solvent induced conformer specific photochemistry of guaiacol. Physical Chemistry Chemical Physics, 2014, 16, 16187.	1.3	41
57	Fragmentation dynamics of the ethyl bromide and ethyl iodide cations: a velocity-map imaging study. Physical Chemistry Chemical Physics, 2014, 16, 2167-2178.	1.3	15
58	Symmetry matters: photodissociation dynamics of symmetrically versus asymmetrically substituted phenols. Physical Chemistry Chemical Physics, 2014, 16, 588-598.	1.3	38
59	Towards Understanding Photodegradation Pathways in Lignins: The Role of Intramolecular Hydrogen Bonding in Excited States. Journal of Physical Chemistry Letters, 2014, 5, 2138-2143.	2.1	22
60	Ab Initio Study of Potential Ultrafast Internal Conversion Routes in Oxybenzone, Caffeic Acid, and Ferulic Acid: Implications for Sunscreens. Journal of Physical Chemistry A, 2014, 118, 11999-12010.	1.1	90
61	Oâ€“H bond fission in 4-substituted phenols: S1 state predissociation viewed in a Hammett-like framework. Chemical Science, 2013, 4, 2434.	3.7	46
62	Exploring quantum phenomena and vibrational control in Ïƒ* mediated photochemistry. Chemical Science, 2013, 4, 993-1001.	3.7	67
63	UV Photodissociation of Pyrroles: Symmetry and Substituent Effects. Journal of Physical Chemistry A, 2013, 117, 12067-12074.	1.1	26
64	Competing 1Ï€Ïƒ* mediated dynamics in mequinol: Oâ€“H versus Oâ€“CH3 photodissociation pathways. Physical Chemistry Chemical Physics, 2012, 14, 13415.	1.3	27
65	Photofragmentation Dynamics in Solution Probed by Transient IR Absorption Spectroscopy: Ï€Ïƒ*-Mediated Bond Cleavage in p-Methylthiophenol and p-Methylthioanisole. Journal of Physical Chemistry Letters, 2012, 3, 3715-3720.	2.1	20