Spiridoula Matsika

List of Publications by Year
in descending order

119	3,969	109321	149698
papers	citations	35 h-index	56 g-index

121	121	121	2890
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Radiationless Decay of Excited States of Uracil through Conical Intersections. Journal of Physical Chemistry A, 2004, 108, 7584-7590.	2.5	264
2	Nonadiabatic Events and Conical Intersections. Annual Review of Physical Chemistry, 2011, 62, 621-643.	10.8	253
3	Three-State Conical Intersections in Nucleic Acid Bases. Journal of Physical Chemistry A, 2005, 109, 7538-7545.	2.5	130
4	Radiationless Decay Mechanism of Cytosine:â€‰ An Ab Initio Study with Comparisons to the Fluorescent Analogue 5-Methyl-2-pyrimidinone. Journal of Physical Chemistry A, 2007, 111, 2650-2661.	2.5	129
5	On the Electronically Excited States of Uracil. Journal of Physical Chemistry A, 2008, 112, 9983-9992.	2.5	115
6	Three-state conical intersections in cytosine and pyrimidinone bases. Journal of Chemical Physics, 2008, 128, 215102.	3.0	110
7	Electronic Spectrum of the NpO22+ and NpO2+ Ions. Journal of Physical Chemistry A, 2000, 104, 4064-4068.	2.5	87
8	Two-Dimensional Ultrafast Fourier Transform Spectroscopy in the Deep Ultraviolet. Optics Express, 2009, 17, 18788.	3.4	87
9	Actinyl Ions in Cs2UO2Cl4. Journal of Physical Chemistry A, 2001, 105, 637-645.	2.5	86
10	What We Can Learn from the Norms of One-Particle Density Matrices, and What We Canâ€™t: Some Results for Interstate Properties in Model Singlet Fission Systems. Journal of Physical Chemistry A, 2014, 118, 11943-11955.	2.5	80
11	Beyond Two-State Conical Intersections. Three-State Conical Intersections in Low Symmetry Molecules:â€‰ the Allyl Radical. Journal of the American Chemical Society, 2003, 125, 10672-10676.	13.7	77
12	Intensities in the Spectra of Actinyl Ions. Journal of Physical Chemistry A, 2000, 104, 11983-11992.	2.5	68
13	Accidental conical intersections of three states of the same symmetry. I. Location and relevance. Journal of Chemical Physics, 2002, 117, 6907-6910.	3.0	68
14	Dyson norms in XUV and strong-field ionization of polyatomics: Cytosine and uracil. Physical Review A, 2012, 86, .	2.5	65
15	A Benchmark of Excitonic Couplings Derived from Atomic Transition Charges. Journal of Physical Chemistry B, 2013, 117, 2032-2044.	2.6	65
16	Electronic Structure Methods for the Description of Nonadiabatic Effects and Conical Intersections. Chemical Reviews, 2021, 121, 9407-9449.	47.7	61
17	Closed-loop learning control of isomerization using shaped ultrafast laser pulses in the deep ultraviolet. Journal of Chemical Physics, 2009, 130, 134311.	3.0	58
18	Solvatochromic Shifts of Uracil and Cytosine Using a Combined Multireference Configuration Interaction/Molecular Dynamics Approach and the Fragment Molecular Orbital Method. Journal of Physical Chemistry A, 2009, 113, 12396-12403.	2.5	58

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19	Pathways for Fluorescence Quenching in 2-Aminopurine Ï€-Stacked with Pyrimidine Nucleobases. Journal of the American Chemical Society, 2011, 133, 6799-6808.	13.7	49
20	Substituent Effects on the Absorption and Fluorescence Properties of Anthracene. Journal of Physical Chemistry A, 2017, 121, 1213-1222.	2.5	49
21	Conical Intersections of Three Electronic States Affect the Ground State of Radical Species with Little or No Symmetry:Â Pyrazolyl. Journal of the American Chemical Society, 2003, 125, 12428-12429.	13.7	47
22	Conical Intersections in Molecular Systems. Reviews in Computational Chemistry, 2007, , 83-124.	1.5	47
23	Excited-State Energies and Electronic Couplings of DNA Base Dimers. Journal of Physical Chemistry B, 2010, 114, 1674-1683.	2.6	47
24	Two-Dimensional Fourier Transform Spectroscopy of Adenine and Uracil Using Shaped Ultrafast Laser Pulses in the Deep UV. Journal of Physical Chemistry A, 2012, 116, 2654-2661.	2.5	46
25	Ultrafast Relaxation Dynamics of Uracil Probed via Strong Field Dissociative Ionization. Journal of Physical Chemistry A, 2013, 117, 12796-12801.	2.5	46
26	Calculations of non-adiabatic couplings within equation-of-motion coupled-cluster framework: Theory, implementation, and validation against multi-reference methods. Journal of Chemical Physics, 2018, 148, 044103.	3.0	44
27	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
28	Cytosine in Context:â€‰ A Theoretical Study of Substituent Effects on the Excitation Energies of 2-Pyrimidinone Derivatives. Journal of Physical Chemistry A, 2007, 111, 8708-8716.	2.5	40
29	Excited electronic states and photophysics of uracilâ€“water complexes. Chemical Physics, 2008, 347, 393-404.	1.9	40
30	Following Ultrafast Radiationless Relaxation Dynamics With Strong Field Dissociative Ionization: A Comparison Between Adenine, Uracil, and Cytosine. IEEE Journal of Selected Topics in Quantum Electronics, 2012, 18, 187-194.	2.9	39
31	An Ab Initio Study of Substituent Effects on the Excited States of Purine Derivatives. Journal of Physical Chemistry A, 2008, 112, 12485-12491.	2.5	38
32	Excimers and Exciplexes in Photoinitiated Processes of Oligonucleotides. Journal of Physical Chemistry Letters, 2016, 7, 976-984.	4.6	38
33	Quantitative detection of singlet O_2 by cavity-enhanced absorption. Optics Letters, 2004, 29, 1066.	3.3	36
34	Intersystem crossing in the exit channel. Nature Chemistry, 2019, 11, 123-128.	13.6	36
35	On the Accessibility to Conical Intersections in Purines: Hypoxanthine and its Singly Protonated and Deprotonated Forms. Journal of the American Chemical Society, 2012, 134, 7820-7829.	13.7	35
36	Controlling Photorelaxation in Uracil with Shaped Laser Pulses: AÂTheoretical Assessment. Journal of the American Chemical Society, 2017, 139, 5061-5066.	13.7	35

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37	Role of Excitonic Coupling and Charge-Transfer States in the Absorption and CD Spectra of Adenine-Based Oligonucleotides Investigated through QM/MM Simulations. Journal of Physical Chemistry A, 2014, 118, 12021-12030.	2.5	34
38	Surface hopping investigation of the relaxation dynamics in radical cations. Journal of Chemical Physics, 2016, 144, 034301.	3.0	33
39	Fragmentation Pathways in the Uracil Radical Cation. Journal of Physical Chemistry A, 2012, 116, 9217-9227.	2.5	32
40	Exciplexes and conical intersections lead to fluorescence quenching in Ï€-stacked dimers of 2-aminopurine with natural purine nucleobases. Photochemical and Photobiological Sciences, 2013, 12, 1387.	2.9	32
41	Intersecting Conical Intersection Seams:â€‰ Their Location, Representation, and Effect on Local Topography. Journal of Physical Chemistry A, 2002, 106, 2580-2591.	2.5	31
42	Contrasting Photophysical Properties of Star-Shaped vs Linear Perylene Diimide Complexes. Journal of the American Chemical Society, 2013, 135, 3056-3066.	13.7	31
43	Excited-State Tautomerization of Gas-Phase Cytosine. Journal of Physical Chemistry A, 2013, 117, 12165-12174.	2.5	31
44	Two- and three-state conical intersections in the uracil cation. Chemical Physics, 2008, 349, 356-362.	1.9	30
45	Comparative study of methodologies for calculating metastable states of small to medium-sized molecules. Journal of Chemical Physics, 2019, 151, 244104.	3.0	30
46	Neutral-Ionic State Correlations in Strong-Field Molecular Ionization. Physical Review Letters, 2012, 109, 203007.	7.8	29
47	On the effects of spin-orbit coupling on conical intersection seams in molecules with an odd number of electrons. I. Locating the seam. Journal of Chemical Physics, 2001, 115, 2038-2050.	3.0	28
48	Inclusion of second-order correlation effects for the ground and singly-excited states suitable for the study of conical intersections: The CIS(2) model. Chemical Physics Letters, 2007, 448, 132-137.	2.6	27
49	QM/MM studies reveal pathways leading to the quenching of the formation of thymine dimer photoproduct by flanking bases. Physical Chemistry Chemical Physics, 2015, 17, 9927-9935.	2.8	27
50	Core-excited and shape resonances of uracil. Physical Chemistry Chemical Physics, 2016, 18, 30536-30545.	2.8	27
51	Bonded Excimer Formation in Ï€-Stacked 9-Methyladenine Dimers. Journal of Physical Chemistry A, 2013, 117, 8718-8728.	2.5	25
52	Change in Electronic Structure upon Optical Excitation of 8-Vinyladenosine: An Experimental and Theoretical Study. Journal of Physical Chemistry A, 2010, 114, 256-267.	2.5	24
53	Spin-orbit coupling and conical intersections in molecules with an odd number of electrons. III. A perturbative determination of the electronic energies, derivative couplings and a rigorous diabatic representation near a conical intersection. Journal of Chemical Physics, 2002, 116, 2825-2835.	3.0	23
54	Photodissociation of the vinoxy radical through conical, and avoided, intersections. Journal of Chemical Physics, 2002, 117, 7198-7206.	3.0	23

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55	Photophysical pathways of cytosine in aqueous solution. Physical Chemistry Chemical Physics, 2010, 12, 5024.	2.8	23
56	Measurement of an Electronic Resonance in a Ground-State, Gas-Phase Acetophenone Cation via Strong-Field Mass Spectrometry. Journal of Physical Chemistry Letters, 2013, 4, 1587-1591.	4.6	23
57	Photoelectron Spectrum and Dynamics of the Uracil Cation. Journal of Physical Chemistry A, 2015, 119, 866-875.	2.5	23
58	Coexistence of Different Electronâ€Transfer Mechanisms in the DNA Repair Process by Photolyase. Chemistry - A European Journal, 2016, 22, 11371-11381.	3.3	23
59	6MAP, a Fluorescent Adenine Analogue, Is a Probe of Base Flipping by DNA Photolyase. Journal of Physical Chemistry B, 2007, 111, 10615-10625.	2.6	22
60	Spinâ^'Orbit Splittings in Mg+â^'Neutral Complexes. Journal of Physical Chemistry A, 1998, 102, 1652-1656.	2.5	20
61	On the effects of spinâ€“orbit coupling on conical intersection seams in molecules with an odd number of electrons. II. Characterizing the local topography of the seam. Journal of Chemical Physics, 2001, 115, 5066-5075.	3.0	20
62	Combining dissociative ionization pumpâ€“probe spectroscopy and ab initio calculations to interpret dynamics and control through conical intersections. Faraday Discussions, 2011, 153, 247.	3.2	20
63	Introduction: Theoretical Modeling of Excited State Processes. Chemical Reviews, 2018, 118, 6925-6926.	47.7	20
64	The Fluorescence Mechanism of 5-Methyl-2-Pyrimidinone: An Ab Initio Study of a Fluorescent Pyrimidine Analog.. Photochemistry and Photobiology, 2006, 83, 611-24.	2.5	19
65	High-Multiplicity Natural Orbitals in Multireference Configuration Interaction for Excited States. Journal of Chemical Theory and Computation, 2012, 8, 509-517.	5.3	19
66	Electronic Resonances of Nucleobases Using Stabilization Methods. Journal of Physical Chemistry A, 2018, 122, 4048-4057.	2.5	19
67	Spinâ^'Orbit Coupling and Conical Intersections. IV. A Perturbative Determination of the Electronic Energies, Derivative Couplings, and a Rigorous Diabatic Representation near a Conical Intersection. The General Caseâ€. Journal of Physical Chemistry B, 2002, 106, 8108-8116.	2.6	18
68	Excited Electronic States of the Cyclic Isomers of O3 and SO2. Journal of Physical Chemistry A, 2005, 109, 11304-11311.	2.5	18
69	Combined Multireference Configuration Interaction/ Molecular Dynamics Approach for Calculating Solvatochromic Shifts:â€‰ Application to the nO â†' Ï€* Electronic Transition of Formaldehyde. Journal of Physical Chemistry A, 2006, 110, 12035-12043.	2.5	18
70	Ultrafast Excited-State Dynamics and Vibrational Cooling of 8-Oxo-7,8-dihydro-2â€²-deoxyguanosine in D₂O. Journal of Physical Chemistry A, 2013, 117, 12851-12857.	2.5	18
71	Measurement of Ionic Resonances in Alkyl Phenyl Ketone Cations via Infrared Strong Field Mass Spectrometry. Journal of Physical Chemistry A, 2013, 117, 12374-12381.	2.5	18
72	Strong Field Adiabatic Ionization Prepares a Launch State for Coherent Control. Journal of Physical Chemistry Letters, 2014, 5, 4305-4309.	4.6	18

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73	State-resolved distribution of OH Xâ€‰Î2 products arising from electronic quenching of OH Aâ€‰Î£2+ by N2. Journal of Chemical Physics, 2009, 130, 104307.	3.0	17
74	High-Multiplicity Natural Orbitals in Multireference Configuration Interaction for Excited State Potential Energy Surfaces. Journal of Physical Chemistry A, 2013, 117, 7421-7430.	2.5	17
75	Theoretical Investigation of Positional Substitution and Solvent Effects on n-Cyanoindole Fluorescent Probes. Journal of Physical Chemistry B, 2019, 123, 7424-7435.	2.6	17
76	2-Aminopurine Excited State Electronic Structure Measured by Stark Spectroscopy. Journal of Physical Chemistry B, 2008, 112, 1789-1795.	2.6	16
77	Photophysical properties of pyrrolocytosine, a cytosine fluorescent base analogue. Physical Chemistry Chemical Physics, 2016, 18, 20189-20198.	2.8	16
78	Strong-field- versus weak-field-ionization pump-probe spectroscopy. Physical Review A, 2018, 98, .	2.5	16
79	Exact-Factorization-Based Surface Hopping for Multistate Dynamics. Journal of Physical Chemistry Letters, 2022, 13, 1785-1790.	4.6	16
80	Strong-Field Molecular Ionization from Multiple Orbitals. Physical Review X, 2011, 1, .	8.9	15
81	Controlling the dissociation dynamics of acetophenone radical cation through excitation of ground and excited state wavepackets. Journal of Physics B: Atomic, Molecular and Optical Physics, 2015, 48, 164002.	1.5	15
82	Photophysical deactivation pathways in adenine oligonucleotides. Physical Chemistry Chemical Physics, 2015, 17, 31073-31083.	2.8	15
83	Effect of dynamic correlation on the ultrafast relaxation of uracil in the gas phase. Faraday Discussions, 2021, 228, 266-285.	3.2	15
84	The origin of fluorescence in DNA thio-analogues. Chemical Physics, 2018, 515, 434-440.	1.9	14
85	Radical cation spectroscopy of substituted alkyl phenyl ketones via tunnel ionization. Chemical Physics, 2014, 442, 81-85.	1.9	13
86	Photochemical Formation of Cyclobutane Pyrimidine Dimers in DNA through Electron Transfer from a Flanking Base. ChemPhysChem, 2018, 19, 1568-1571.	2.1	13
87	Benchmarking Quantum Mechanical Methods for the Description of Charge-Transfer States in Ï€-Stacked Nucleobases. Journal of Chemical Theory and Computation, 2021, 17, 376-387.	5.3	13
88	Time Resolved Photoelectron Spectroscopy as a Test of Electronic Structure and Nonadiabatic Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 5099-5104.	4.6	13
89	Accurate Modeling of Excitonic Coupling in Cyanine Dye Cy3. Journal of Physical Chemistry A, 2021, 125, 7852-7866.	2.5	13
90	Conical intersections and the nonadiabatic reactions H2O+O(3P)â†”OH(Aâ€Š2Î£+)+OH(Xâ€Š2Î). Journal of Chemical Physics, 2002, 117, 3733-3740.	3.0	12

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91	Angleâ€Resolved Strongâ€Field Ionization of Polyatomic Molecules: More than the Orbitals Matters. ChemPhysChem, 2013, 14, 1451-1455.	2.1	12
92	Excited State Relaxation of Neutral and Basic 8-Oxoguanine. Journal of Physical Chemistry B, 2015, 119, 8293-8301.	2.6	12
93	Conformational and electronic effects on the formation of anti cyclobutane pyrimidine dimers in G-quadruplex structures. Physical Chemistry Chemical Physics, 2017, 19, 3325-3336.	2.8	12
94	Role of charge transfer states into the formation of cyclobutane pyrimidine dimers in DNA. Faraday Discussions, 2019, 216, 507-519.	3.2	12
95	Mechanisms of H and CO loss from the uracil nucleobase following low energy electron irradiation. Physical Chemistry Chemical Physics, 2017, 19, 17233-17241.	2.8	11
96	The influence of excited state topology on wavepacket delocalization in the relaxation of photoexcited polyatomic molecules. Journal of Chemical Physics, 2012, 137, 22A537.	3.0	10
97	Mechanistic insights into photoinduced damage of DNA and RNA nucleobases in the gas phase and in bulk solution. Faraday Discussions, 2018, 207, 329-350.	3.2	10
98	Electron correlation in channel-resolved strong-field molecular double ionization. Physical Review A, 2019, 100, .	2.5	10
99	Ultrafast internal conversion dynamics of highly excited pyrrole studied with VUV/UV pump probe spectroscopy. Journal of Chemical Physics, 2017, 146, 064306.	3.0	9
100	Excited state dynamics of cis,cis-1,3-cyclooctadiene: Non-adiabatic trajectory surface hopping. Journal of Chemical Physics, 2020, 152, 174302.	3.0	9
101	Modeling solvation effects on absorption and fluorescence spectra of indole in aqueous solution. Journal of Chemical Physics, 2021, 154, 064104.	3.0	9
102	Conical Intersections and the Spin-Orbit Interaction. Advances in Chemical Physics, 2003, , 557-581.	0.3	8
103	Molecular Double Ionization Using Strong Field Few-Cycle Laser Pulses. Journal of Physical Chemistry A, 2016, 120, 3233-3240.	2.5	8
104	Description of Two-Particle One-Hole Electronic Resonances Using Orbital Stabilization Methods. Journal of Physical Chemistry A, 2020, 124, 9011-9020.	2.5	8
105	Excited state dynamics of cis,cis-1,3-cyclooctadiene: UV pump VUV probe time-resolved photoelectron spectroscopy. Journal of Chemical Physics, 2020, 153, 074301.	3.0	8
106	Modeling the Ultrafast Electron Attachment Dynamics of Solvated Uracil. Journal of Physical Chemistry A, 2021, 125, 6995-7003.	2.5	8
107	Modeling the Electronic Absorption Spectra of the Indocarbocyanine Cy3. Molecules, 2022, 27, 4062.	3.8	8
108	Vibrationally assisted below-threshold ionization. Physical Review A, 2017, 95, .	2.5	7

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109	Projected Complex Absorbing Potential Multireference Configuration Interaction Approach for Shape and Feshbach Resonances. Journal of Chemical Theory and Computation, 0, , .	5.3	7
110	Origins of Photodamage in Pheomelanin Constituents: Photochemistry of 4-Hydroxybenzothiazole. Journal of Physical Chemistry A, 2018, 122, 1986-1993.	2.5	5
111	Understanding the Interplay between the Nonvalence and Valence States of the Uracil Anion upon Monohydration. Journal of Physical Chemistry A, 2020, 124, 9237-9243.	2.5	5
112	Theoretical studies of the excited states of p-cyanophenylalanine and comparisons with the natural amino acids phenylalanine and tyrosine. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	4
113	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.	2.8	3
114	Stabilization of the Triplet Biradical Intermediate of 5â€²Methylcytosine Enhances Cyclobutane Pyrimidine Dimer (CPD) Formation in DNA. Chemistry - A European Journal, 2020, 26, 14181-14186.	3.3	3
115	A Unique QP Partitioning and Siegert Width Using Real-Valued Continuum-Remover Potential. Journal of Chemical Theory and Computation, 2022, 18, 2863-2874.	5.3	3
116	Three-State Conical Intersections. Advanced Series in Physical Chemistry, 2011, , 83-116.	1.5	2
117	Quadruple coincidence measurement of electron correlation in strong-field molecular double ionization. Physical Review A, 2018, 97, .	2.5	2
118	Conformer-Specific Dissociation Dynamics in Dimethyl Methylphosphonate Radical Cation. Molecules, 2022, 27, 2269.	3.8	1
119	Developments in ultrafast spectroscopy. Physical Chemistry Chemical Physics, 2022, , .	2.8	1