Spiridoula Matsika

List of Publications by Year
in descending order

119	3,969	125106	169272
papers	citations	35 h-index	56 g-index

121	121	121	3262
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Exact-Factorization-Based Surface Hopping for Multistate Dynamics. Journal of Physical Chemistry Letters, 2022, 13, 1785-1790.	2.1	16
2	Conformer-Specific Dissociation Dynamics in Dimethyl Methylphosphonate Radical Cation. Molecules, 2022, 27, 2269.	1.7	1
3	A Unique QP Partitioning and Siegert Width Using Real-Valued Continuum-Remover Potential. Journal of Chemical Theory and Computation, 2022, 18, 2863-2874.	2.3	3
4	Developments in ultrafast spectroscopy. Physical Chemistry Chemical Physics, 2022, , .	1.3	1
5	Modeling the Electronic Absorption Spectra of the Indocarbocyanine Cy3. Molecules, 2022, 27, 4062.	1.7	8
6	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.	2.3	13
7	Effect of dynamic correlation on the ultrafast relaxation of uracil in the gas phase. Faraday Discussions, 2021, 228, 266-285.	1.6	15
8	Modeling solvation effects on absorption and fluorescence spectra of indole in aqueous solution. Journal of Chemical Physics, 2021, 154, 064104.	1.2	9
9	Time Resolved Photoelectron Spectroscopy as a Test of Electronic Structure and Nonadiabatic Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 5099-5104.	2.1	13
10	Electronic Structure Methods for the Description of Nonadiabatic Effects and Conical Intersections. Chemical Reviews, 2021, 121, 9407-9449.	23.0	61
11	Modeling the Ultrafast Electron Attachment Dynamics of Solvated Uracil. Journal of Physical Chemistry A, 2021, 125, 6995-7003.	1.1	8
12	Accurate Modeling of Excitonic Coupling in Cyanine Dye Cy3. Journal of Physical Chemistry A, 2021, 125, 7852-7866.	1.1	13
13	Description of Two-Particle One-Hole Electronic Resonances Using Orbital Stabilization Methods. Journal of Physical Chemistry A, 2020, 124, 9011-9020.	1.1	8
14	Understanding the Interplay between the Nonvalence and Valence States of the Uracil Anion upon Monohydration. Journal of Physical Chemistry A, 2020, 124, 9237-9243.	1.1	5
15	Stabilization of the Triplet Biradical Intermediate of 5â€Methylcytosine Enhances Cyclobutane Pyrimidine Dimer (CPD) Formation in DNA. Chemistry - A European Journal, 2020, 26, 14181-14186.	1.7	3
16	Excited state dynamics of cis,cis-1,3-cyclooctadiene: UV pump VUV probe time-resolved photoelectron spectroscopy. Journal of Chemical Physics, 2020, 153, 074301.	1.2	8
17	Excited state dynamics of cis,cis-1,3-cyclooctadiene: Non-adiabatic trajectory surface hopping. Journal of Chemical Physics, 2020, 152, 174302.	1.2	9
18	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	1.2	42

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19	Theoretical Investigation of Positional Substitution and Solvent Effects on n-Cyanoindole Fluorescent Probes. Journal of Physical Chemistry B, 2019, 123, 7424-7435.	1.2	17
20	Electron correlation in channel-resolved strong-field molecular double ionization. Physical Review A, 2019, 100, .	1.0	10
21	Role of charge transfer states into the formation of cyclobutane pyrimidine dimers in DNA. Faraday Discussions, 2019, 216, 507-519.	1.6	12
22	Comparative study of methodologies for calculating metastable states of small to medium-sized molecules. Journal of Chemical Physics, 2019, 151, 244104.	1.2	30
23	Intersystem crossing in the exit channel. Nature Chemistry, 2019, 11, 123-128.	6.6	36
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	Quadruple coincidence measurement of electron correlation in strong-field molecular double ionization. Physical Review A, 2018, 97, .	1.0	2
26	Electronic Resonances of Nucleobases Using Stabilization Methods. Journal of Physical Chemistry A, 2018, 122, 4048-4057.	1.1	19
27	Photochemical Formation of Cyclobutane Pyrimidine Dimers in DNA through Electron Transfer from a Flanking Base. ChemPhysChem, 2018, 19, 1568-1571.	1.0	13
28	Origins of Photodamage in Pheomelanin Constituents: Photochemistry of 4-Hydroxybenzothiazole. Journal of Physical Chemistry A, 2018, 122, 1986-1993.	1.1	5
29	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.	1.2	44
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	Strong-field- versus weak-field-ionization pump-probe spectroscopy. Physical Review A, 2018, 98, .	1.0	16
32	The origin of fluorescence in DNA thio-analogues. Chemical Physics, 2018, 515, 434-440.	0.9	14
33	Introduction: Theoretical Modeling of Excited State Processes. Chemical Reviews, 2018, 118, 6925-6926.	23.0	20
34	Substituent Effects on the Absorption and Fluorescence Properties of Anthracene. Journal of Physical Chemistry A, 2017, 121, 1213-1222.	1.1	49
35	Ultrafast internal conversion dynamics of highly excited pyrrole studied with VUV/UV pump probe spectroscopy. Journal of Chemical Physics, 2017, 146, 064306.	1.2	9
36	Controlling Photorelaxation in Uracil with Shaped Laser Pulses: AÂTheoretical Assessment. Journal of the American Chemical Society, 2017, 139, 5061-5066.	6.6	35

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37	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
38	Conformational and electronic effects on the formation of anti cyclobutane pyrimidine dimers in G-quadruplex structures. Physical Chemistry Chemical Physics, 2017, 19, 3325-3336.	1.3	12
39	Vibrationally assisted below-threshold ionization. Physical Review A, 2017, 95, .	1.0	7
40	Surface hopping investigation of the relaxation dynamics in radical cations. Journal of Chemical Physics, 2016, 144, 034301.	1.2	33
41	Photophysical properties of pyrrolocytosine, a cytosine fluorescent base analogue. Physical Chemistry Chemical Physics, 2016, 18, 20189-20198.	1.3	16
42	Coexistence of Different Electronâ€Transfer Mechanisms in the DNA Repair Process by Photolyase. Chemistry - A European Journal, 2016, 22, 11371-11381.	1.7	23
43	Core-excited and shape resonances of uracil. Physical Chemistry Chemical Physics, 2016, 18, 30536-30545.	1.3	27
44	Excimers and Exciplexes in Photoinitiated Processes of Oligonucleotides. Journal of Physical Chemistry Letters, 2016, 7, 976-984.	2.1	38
45	Molecular Double Ionization Using Strong Field Few-Cycle Laser Pulses. Journal of Physical Chemistry A, 2016, 120, 3233-3240.	1.1	8
46	Excited State Relaxation of Neutral and Basic 8-Oxoguanine. Journal of Physical Chemistry B, 2015, 119, 8293-8301.	1.2	12
47	Photoelectron Spectrum and Dynamics of the Uracil Cation. Journal of Physical Chemistry A, 2015, 119, 866-875.	1.1	23
48	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.	0.6	15
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.	1.3	27
50	Photophysical deactivation pathways in adenine oligonucleotides. Physical Chemistry Chemical Physics, 2015, 17, 31073-31083.	1.3	15
51	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.	1.1	34
52	Strong Field Adiabatic Ionization Prepares a Launch State for Coherent Control. Journal of Physical Chemistry Letters, 2014, 5, 4305-4309.	2.1	18
53	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.	1.1	80
54	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.	0.5	4

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55	Radical cation spectroscopy of substituted alkyl phenyl ketones via tunnel ionization. Chemical Physics, 2014, 442, 81-85.	0.9	13
56	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.	1.1	18
57	High-Multiplicity Natural Orbitals in Multireference Configuration Interaction for Excited State Potential Energy Surfaces. Journal of Physical Chemistry A, 2013, 117, 7421-7430.	1.1	17
58	Contrasting Photophysical Properties of Star-Shaped vs Linear Perylene Diimide Complexes. Journal of the American Chemical Society, 2013, 135, 3056-3066.	6.6	31
59	A Benchmark of Excitonic Couplings Derived from Atomic Transition Charges. Journal of Physical Chemistry B, 2013, 117, 2032-2044.	1.2	65
60	Angleâ€Resolved Strongâ€Field Ionization of Polyatomic Molecules: More than the Orbitals Matters. ChemPhysChem, 2013, 14, 1451-1455.	1.0	12
61	Bonded Excimer Formation in Ï€-Stacked 9-Methyladenine Dimers. Journal of Physical Chemistry A, 2013, 117, 8718-8728.	1.1	25
62	Excited-State Tautomerization of Gas-Phase Cytosine. Journal of Physical Chemistry A, 2013, 117, 12165-12174.	1.1	31
63	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.	2.1	23
64	Measurement of Ionic Resonances in Alkyl Phenyl Ketone Cations via Infrared Strong Field Mass Spectrometry. Journal of Physical Chemistry A, 2013, 117, 12374-12381.	1.1	18
65	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.	1.6	32
66	Ultrafast Relaxation Dynamics of Uracil Probed via Strong Field Dissociative Ionization. Journal of Physical Chemistry A, 2013, 117, 12796-12801.	1.1	46
67	Neutral-Ionic State Correlations in Strong-Field Molecular Ionization. Physical Review Letters, 2012, 109, 203007.	2.9	29
68	The influence of excited state topology on wavepacket delocalization in the relaxation of photoexcited polyatomic molecules. Journal of Chemical Physics, 2012, 137, 22A537.	1.2	10
69	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.	1.1	46
70	Dyson norms in XUV and strong-field ionization of polyatomics: Cytosine and uracil. Physical Review A, 2012, 86, .	1.0	65
71	Fragmentation Pathways in the Uracil Radical Cation. Journal of Physical Chemistry A, 2012, 116, 9217-9227.	1.1	32
72	High-Multiplicity Natural Orbitals in Multireference Configuration Interaction for Excited States. Journal of Chemical Theory and Computation, 2012, 8, 509-517.	2.3	19

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73	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.	6.6	35
74	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.	1.9	39
75	Combining dissociative ionization pumpâ€“probe spectroscopy and ab initio calculations to interpret dynamics and control through conical intersections. Faraday Discussions, 2011, 153, 247.	1.6	20
76	Three-State Conical Intersections. Advanced Series in Physical Chemistry, 2011, , 83-116.	1.5	2
77	Nonadiabatic Events and Conical Intersections. Annual Review of Physical Chemistry, 2011, 62, 621-643.	4.8	253
78	Strong-Field Molecular Ionization from Multiple Orbitals. Physical Review X, 2011, 1, .	2.8	15
79	Pathways for Fluorescence Quenching in 2-Aminopurine Ï€-Stacked with Pyrimidine Nucleobases. Journal of the American Chemical Society, 2011, 133, 6799-6808.	6.6	49
80	Change in Electronic Structure upon Optical Excitation of 8-Vinyladenosine: An Experimental and Theoretical Study. Journal of Physical Chemistry A, 2010, 114, 256-267.	1.1	24
81	Excited-State Energies and Electronic Couplings of DNA Base Dimers. Journal of Physical Chemistry B, 2010, 114, 1674-1683.	1.2	47
82	Photophysical pathways of cytosine in aqueous solution. Physical Chemistry Chemical Physics, 2010, 12, 5024.	1.3	23
83	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.	1.2	17
84	Closed-loop learning control of isomerization using shaped ultrafast laser pulses in the deep ultraviolet. Journal of Chemical Physics, 2009, 130, 134311.	1.2	58
85	Two-Dimensional Ultrafast Fourier Transform Spectroscopy in the Deep Ultraviolet. Optics Express, 2009, 17, 18788.	1.7	87
86	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.	1.1	58
87	Excited electronic states and photophysics of uracilâ€“water complexes. Chemical Physics, 2008, 347, 393-404.	0.9	40
88	Two- and three-state conical intersections in the uracil cation. Chemical Physics, 2008, 349, 356-362.	0.9	30
89	Three-state conical intersections in cytosine and pyrimidinone bases. Journal of Chemical Physics, 2008, 128, 215102.	1.2	110
90	On the Electronically Excited States of Uracil. Journal of Physical Chemistry A, 2008, 112, 9983-9992.	1.1	115

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91	2-Aminopurine Excited State Electronic Structure Measured by Stark Spectroscopy. Journal of Physical Chemistry B, 2008, 112, 1789-1795.	1.2	16
92	An Ab Initio Study of Substituent Effects on the Excited States of Purine Derivatives. Journal of Physical Chemistry A, 2008, 112, 12485-12491.	1.1	38
93	Conical Intersections in Molecular Systems. Reviews in Computational Chemistry, 2007, , 83-124.	1.5	47
94	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.	1.1	40
95	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.	1.1	129
96	6MAP, a Fluorescent Adenine Analogue, Is a Probe of Base Flipping by DNA Photolyase. Journal of Physical Chemistry B, 2007, 111, 10615-10625.	1.2	22
97	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.	1.2	27
98	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.	1.1	18
99	The Fluorescence Mechanism of 5-Methyl-2-Pyrimidinone: An Ab Initio Study of a Fluorescent Pyrimidine Analog.. Photochemistry and Photobiology, 2006, 83, 611-24.	1.3	19
100	Three-State Conical Intersections in Nucleic Acid Bases. Journal of Physical Chemistry A, 2005, 109, 7538-7545.	1.1	130
101	Excited Electronic States of the Cyclic Isomers of O3 and SO2. Journal of Physical Chemistry A, 2005, 109, 11304-11311.	1.1	18
102	Radiationless Decay of Excited States of Uracil through Conical Intersections. Journal of Physical Chemistry A, 2004, 108, 7584-7590.	1.1	264
103	Quantitative detection of singlet O_2 by cavity-enhanced absorption. Optics Letters, 2004, 29, 1066.	1.7	36
104	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.	6.6	47
105	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.	6.6	77
106	Conical Intersections and the Spin-Orbit Interaction. Advances in Chemical Physics, 2003, , 557-581.	0.3	8
107	Conical intersections and the nonadiabatic reactions H2O+O(3P)â†”OH(Aâ€Š2Î£+)+OH(Xâ€Š2Î). Journal of Chemical Physics, 2002, 117, 3733-3740.	1.2	12
108	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.	1.2	23

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109	Photodissociation of the vinoxy radical through conical, and avoided, intersections. Journal of Chemical Physics, 2002, 117, 7198-7206.	1.2	23
110	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.	1.2	18
111	Accidental conical intersections of three states of the same symmetry. I. Location and relevance. Journal of Chemical Physics, 2002, 117, 6907-6910.	1.2	68
112	Intersecting Conical Intersection Seams:â€‰ Their Location, Representation, and Effect on Local Topography. Journal of Physical Chemistry A, 2002, 106, 2580-2591.	1.1	31
113	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.	1.2	28
114	Actinyl Ions in Cs2UO2Cl4. Journal of Physical Chemistry A, 2001, 105, 637-645.	1.1	86
115	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.	1.2	20
116	Intensities in the Spectra of Actinyl Ions. Journal of Physical Chemistry A, 2000, 104, 11983-11992.	1.1	68
117	Electronic Spectrum of the NpO22+ and NpO2+ Ions. Journal of Physical Chemistry A, 2000, 104, 4064-4068.	1.1	87
118	Spinâ˜'Orbit Splittings in Mg+â˜'Neutral Complexes. Journal of Physical Chemistry A, 1998, 102, 1652-1656.	1.1	20
119	Projected Complex Absorbing Potential Multireference Configuration Interaction Approach for Shape and Feshbach Resonances. Journal of Chemical Theory and Computation, 0, , .	2.3	7