

Spiridoula Matsika

List of Publications by Year in descending order

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119
papers

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109321

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121
times ranked

2890
citing authors

#	ARTICLE	IF	CITATIONS
1	Exact-Factorization-Based Surface Hopping for Multistate Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 1785-1790.	4.6	16
2	Conformer-Specific Dissociation Dynamics in Dimethyl Methylphosphonate Radical Cation. <i>Molecules</i> , 2022, 27, 2269.	3.8	1
3	A Unique QP Partitioning and Siegert Width Using Real-Valued Continuum-Remover Potential. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2863-2874.	5.3	3
4	Developments in ultrafast spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2022, , .	2.8	1
5	Modeling the Electronic Absorption Spectra of the Indocarbocyanine Cy3. <i>Molecules</i> , 2022, 27, 4062.	3.8	8
6	Benchmarking Quantum Mechanical Methods for the Description of Charge-Transfer States in π -Stacked Nucleobases. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 376-387.	5.3	13
7	Effect of dynamic correlation on the ultrafast relaxation of uracil in the gas phase. <i>Faraday Discussions</i> , 2021, 228, 266-285.	3.2	15
8	Modeling solvation effects on absorption and fluorescence spectra of indole in aqueous solution. <i>Journal of Chemical Physics</i> , 2021, 154, 064104.	3.0	9
9	Time Resolved Photoelectron Spectroscopy as a Test of Electronic Structure and Nonadiabatic Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 5099-5104.	4.6	13
10	Electronic Structure Methods for the Description of Nonadiabatic Effects and Conical Intersections. <i>Chemical Reviews</i> , 2021, 121, 9407-9449.	47.7	61
11	Modeling the Ultrafast Electron Attachment Dynamics of Solvated Uracil. <i>Journal of Physical Chemistry A</i> , 2021, 125, 6995-7003.	2.5	8
12	Accurate Modeling of Excitonic Coupling in Cyanine Dye Cy3. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7852-7866.	2.5	13
13	Description of Two-Particle One-Hole Electronic Resonances Using Orbital Stabilization Methods. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9011-9020.	2.5	8
14	Understanding the Interplay between the Nonvalence and Valence States of the Uracil Anion upon Monohydration. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9237-9243.	2.5	5
15	Stabilization of the Triplet Biradical Intermediate of 5-Methylcytosine Enhances Cyclobutane Pyrimidine Dimer (CPD) Formation in DNA. <i>Chemistry - A European Journal</i> , 2020, 26, 14181-14186.	3.3	3
16	Excited state dynamics of cis,cis-1,3-cyclooctadiene: UV pump VUV probe time-resolved photoelectron spectroscopy. <i>Journal of Chemical Physics</i> , 2020, 153, 074301.	3.0	8
17	Excited state dynamics of cis,cis-1,3-cyclooctadiene: Non-adiabatic trajectory surface hopping. <i>Journal of Chemical Physics</i> , 2020, 152, 174302.	3.0	9
18	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. <i>Journal of Chemical Physics</i> , 2020, 152, 134110.	3.0	42

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19	Theoretical Investigation of Positional Substitution and Solvent Effects on <i>n</i> -Cyanoindeole Fluorescent Probes. <i>Journal of Physical Chemistry B</i> , 2019, 123, 7424-7435.	2.6	17
20	Electron correlation in channel-resolved strong-field molecular double ionization. <i>Physical Review A</i> , 2019, 100, .	2.5	10
21	Role of charge transfer states into the formation of cyclobutane pyrimidine dimers in DNA. <i>Faraday Discussions</i> , 2019, 216, 507-519.	3.2	12
22	Comparative study of methodologies for calculating metastable states of small to medium-sized molecules. <i>Journal of Chemical Physics</i> , 2019, 151, 244104.	3.0	30
23	Intersystem crossing in the exit channel. <i>Nature Chemistry</i> , 2019, 11, 123-128.	13.6	36
24	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.	2.8	3
25	Quadruple coincidence measurement of electron correlation in strong-field molecular double ionization. <i>Physical Review A</i> , 2018, 97, .	2.5	2
26	Electronic Resonances of Nucleobases Using Stabilization Methods. <i>Journal of Physical Chemistry A</i> , 2018, 122, 4048-4057.	2.5	19
27	Photochemical Formation of Cyclobutane Pyrimidine Dimers in DNA through Electron Transfer from a Flanking Base. <i>ChemPhysChem</i> , 2018, 19, 1568-1571.	2.1	13
28	Origins of Photodamage in Pheomelanin Constituents: Photochemistry of 4-Hydroxybenzothiazole. <i>Journal of Physical Chemistry A</i> , 2018, 122, 1986-1993.	2.5	5
29	Calculations of non-adiabatic couplings within equation-of-motion coupled-cluster framework: Theory, implementation, and validation against multi-reference methods. <i>Journal of Chemical Physics</i> , 2018, 148, 044103.	3.0	44
30	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.	3.2	10
31	Strong-field- versus weak-field-ionization pump-probe spectroscopy. <i>Physical Review A</i> , 2018, 98, .	2.5	16
32	The origin of fluorescence in DNA thio-analogues. <i>Chemical Physics</i> , 2018, 515, 434-440.	1.9	14
33	Introduction: Theoretical Modeling of Excited State Processes. <i>Chemical Reviews</i> , 2018, 118, 6925-6926.	47.7	20
34	Substituent Effects on the Absorption and Fluorescence Properties of Anthracene. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1213-1222.	2.5	49
35	Ultrafast internal conversion dynamics of highly excited pyrrole studied with VUV/UV pump probe spectroscopy. <i>Journal of Chemical Physics</i> , 2017, 146, 064306.	3.0	9
36	Controlling Photorelaxation in Uracil with Shaped Laser Pulses: A Theoretical Assessment. <i>Journal of the American Chemical Society</i> , 2017, 139, 5061-5066.	13.7	35

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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.	2.8	11
38	Conformational and electronic effects on the formation of anti cyclobutane pyrimidine dimers in G-quadruplex structures. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 3325-3336.	2.8	12
39	Vibrationally assisted below-threshold ionization. <i>Physical Review A</i> , 2017, 95, .	2.5	7
40	Surface hopping investigation of the relaxation dynamics in radical cations. <i>Journal of Chemical Physics</i> , 2016, 144, 034301.	3.0	33
41	Photophysical properties of pyrrolocytosine, a cytosine fluorescent base analogue. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 20189-20198.	2.8	16
42	Coexistence of Different Electron-Transfer Mechanisms in the DNA Repair Process by Photolyase. <i>Chemistry - A European Journal</i> , 2016, 22, 11371-11381.	3.3	23
43	Core-excited and shape resonances of uracil. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30536-30545.	2.8	27
44	Excimers and Exciplexes in Photoinitiated Processes of Oligonucleotides. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 976-984.	4.6	38
45	Molecular Double Ionization Using Strong Field Few-Cycle Laser Pulses. <i>Journal of Physical Chemistry A</i> , 2016, 120, 3233-3240.	2.5	8
46	Excited State Relaxation of Neutral and Basic 8-Oxoguanine. <i>Journal of Physical Chemistry B</i> , 2015, 119, 8293-8301.	2.6	12
47	Photoelectron Spectrum and Dynamics of the Uracil Cation. <i>Journal of Physical Chemistry A</i> , 2015, 119, 866-875.	2.5	23
48	Controlling the dissociation dynamics of acetophenone radical cation through excitation of ground and excited state wavepackets. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2015, 48, 164002.	1.5	15
49	QM/MM studies reveal pathways leading to the quenching of the formation of thymine dimer photoproduct by flanking bases. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 9927-9935.	2.8	27
50	Photophysical deactivation pathways in adenine oligonucleotides. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 31073-31083.	2.8	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. <i>Journal of Physical Chemistry A</i> , 2014, 118, 12021-12030.	2.5	34
52	Strong Field Adiabatic Ionization Prepares a Launch State for Coherent Control. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 4305-4309.	4.6	18
53	What We Can Learn from the Norms of One-Particle Density Matrices, and What We Can't: Some Results for Interstate Properties in Model Singlet Fission Systems. <i>Journal of Physical Chemistry A</i> , 2014, 118, 11943-11955.	2.5	80
54	Theoretical studies of the excited states of p-cyanophenylalanine and comparisons with the natural amino acids phenylalanine and tyrosine. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	1.4	4

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55	Radical cation spectroscopy of substituted alkyl phenyl ketones via tunnel ionization. <i>Chemical Physics</i> , 2014, 442, 81-85.	1.9	13
56	Ultrafast Excited-State Dynamics and Vibrational Cooling of 8-Oxo-7,8-dihydro-2- ϵ -deoxyguanosine in D_2O . <i>Journal of Physical Chemistry A</i> , 2013, 117, 12851-12857.	2.5	18
57	High-Multiplicity Natural Orbitals in Multireference Configuration Interaction for Excited State Potential Energy Surfaces. <i>Journal of Physical Chemistry A</i> , 2013, 117, 7421-7430.	2.5	17
58	Contrasting Photophysical Properties of Star-Shaped vs Linear Perylene Diimide Complexes. <i>Journal of the American Chemical Society</i> , 2013, 135, 3056-3066.	13.7	31
59	A Benchmark of Excitonic Couplings Derived from Atomic Transition Charges. <i>Journal of Physical Chemistry B</i> , 2013, 117, 2032-2044.	2.6	65
60	Angle-Resolved Strong-Field Ionization of Polyatomic Molecules: More than the Orbitals Matters. <i>ChemPhysChem</i> , 2013, 14, 1451-1455.	2.1	12
61	Bonded Excimer Formation in π -Stacked 9-Methyladenine Dimers. <i>Journal of Physical Chemistry A</i> , 2013, 117, 8718-8728.	2.5	25
62	Excited-State Tautomerization of Gas-Phase Cytosine. <i>Journal of Physical Chemistry A</i> , 2013, 117, 12165-12174.	2.5	31
63	Measurement of an Electronic Resonance in a Ground-State, Gas-Phase Acetophenone Cation via Strong-Field Mass Spectrometry. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 1587-1591.	4.6	23
64	Measurement of Ionic Resonances in Alkyl Phenyl Ketone Cations via Infrared Strong Field Mass Spectrometry. <i>Journal of Physical Chemistry A</i> , 2013, 117, 12374-12381.	2.5	18
65	Exciplexes and conical intersections lead to fluorescence quenching in π -stacked dimers of 2-aminopurine with natural purine nucleobases. <i>Photochemical and Photobiological Sciences</i> , 2013, 12, 1387.	2.9	32
66	Ultrafast Relaxation Dynamics of Uracil Probed via Strong Field Dissociative Ionization. <i>Journal of Physical Chemistry A</i> , 2013, 117, 12796-12801.	2.5	46
67	Neutral-Ionic State Correlations in Strong-Field Molecular Ionization. <i>Physical Review Letters</i> , 2012, 109, 203007.	7.8	29
68	The influence of excited state topology on wavepacket delocalization in the relaxation of photoexcited polyatomic molecules. <i>Journal of Chemical Physics</i> , 2012, 137, 22A537.	3.0	10
69	Two-Dimensional Fourier Transform Spectroscopy of Adenine and Uracil Using Shaped Ultrafast Laser Pulses in the Deep UV. <i>Journal of Physical Chemistry A</i> , 2012, 116, 2654-2661.	2.5	46
70	Dyson norms in XUV and strong-field ionization of polyatomics: Cytosine and uracil. <i>Physical Review A</i> , 2012, 86, .	2.5	65
71	Fragmentation Pathways in the Uracil Radical Cation. <i>Journal of Physical Chemistry A</i> , 2012, 116, 9217-9227.	2.5	32
72	High-Multiplicity Natural Orbitals in Multireference Configuration Interaction for Excited States. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 509-517.	5.3	19

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73	On the Accessibility to Conical Intersections in Purines: Hypoxanthine and its Singly Protonated and Deprotonated Forms. <i>Journal of the American Chemical Society</i> , 2012, 134, 7820-7829.	13.7	35
74	Following Ultrafast Radiationless Relaxation Dynamics With Strong Field Dissociative Ionization: A Comparison Between Adenine, Uracil, and Cytosine. <i>IEEE Journal of Selected Topics in Quantum Electronics</i> , 2012, 18, 187-194.	2.9	39
75	Combining dissociative ionization pump-probe spectroscopy and ab initio calculations to interpret dynamics and control through conical intersections. <i>Faraday Discussions</i> , 2011, 153, 247.	3.2	20
76	Three-State Conical Intersections. <i>Advanced Series in Physical Chemistry</i> , 2011, , 83-116.	1.5	2
77	Nonadiabatic Events and Conical Intersections. <i>Annual Review of Physical Chemistry</i> , 2011, 62, 621-643.	10.8	253
78	Strong-Field Molecular Ionization from Multiple Orbitals. <i>Physical Review X</i> , 2011, 1, .	8.9	15
79	Pathways for Fluorescence Quenching in 2-Aminopurine π -Stacked with Pyrimidine Nucleobases. <i>Journal of the American Chemical Society</i> , 2011, 133, 6799-6808.	13.7	49
80	Change in Electronic Structure upon Optical Excitation of 8-Vinyladenosine: An Experimental and Theoretical Study. <i>Journal of Physical Chemistry A</i> , 2010, 114, 256-267.	2.5	24
81	Excited-State Energies and Electronic Couplings of DNA Base Dimers. <i>Journal of Physical Chemistry B</i> , 2010, 114, 1674-1683.	2.6	47
82	Photophysical pathways of cytosine in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 5024.	2.8	23
83	State-resolved distribution of OH \dot{X} products arising from electronic quenching of OH \dot{X}^+ by N ₂ . <i>Journal of Chemical Physics</i> , 2009, 130, 104307.	3.0	17
84	Closed-loop learning control of isomerization using shaped ultrafast laser pulses in the deep ultraviolet. <i>Journal of Chemical Physics</i> , 2009, 130, 134311.	3.0	58
85	Two-Dimensional Ultrafast Fourier Transform Spectroscopy in the Deep Ultraviolet. <i>Optics Express</i> , 2009, 17, 18788.	3.4	87
86	Solvatochromic Shifts of Uracil and Cytosine Using a Combined Multireference Configuration Interaction/Molecular Dynamics Approach and the Fragment Molecular Orbital Method. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12396-12403.	2.5	58
87	Excited electronic states and photophysics of uracil-water complexes. <i>Chemical Physics</i> , 2008, 347, 393-404.	1.9	40
88	Two- and three-state conical intersections in the uracil cation. <i>Chemical Physics</i> , 2008, 349, 356-362.	1.9	30
89	Three-state conical intersections in cytosine and pyrimidinone bases. <i>Journal of Chemical Physics</i> , 2008, 128, 215102.	3.0	110
90	On the Electronically Excited States of Uracil. <i>Journal of Physical Chemistry A</i> , 2008, 112, 9983-9992.	2.5	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.	2.6	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.	2.5	38
93	Conical Intersections in Molecular Systems. Reviews in Computational Chemistry, 2007, , 83-124.	1.5	47
94	Cytosine in Context: 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
95	Radiationless Decay Mechanism of Cytosine: 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
96	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
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.	2.6	27
98	Combined Multireference Configuration Interaction/ Molecular Dynamics Approach for Calculating Solvatochromic Shifts: Application to the nO $\hat{\rightarrow}$ $\hat{\leftarrow}$ * Electronic Transition of Formaldehyde. Journal of Physical Chemistry A, 2006, 110, 12035-12043.	2.5	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.	2.5	19
100	Three-State Conical Intersections in Nucleic Acid Bases. Journal of Physical Chemistry A, 2005, 109, 7538-7545.	2.5	130
101	Excited Electronic States of the Cyclic Isomers of O3 and SO2. Journal of Physical Chemistry A, 2005, 109, 11304-11311.	2.5	18
102	Radiationless Decay of Excited States of Uracil through Conical Intersections. Journal of Physical Chemistry A, 2004, 108, 7584-7590.	2.5	264
103	Quantitative detection of singlet O ₂ by cavity-enhanced absorption. Optics Letters, 2004, 29, 1066.	3.3	36
104	Conical Intersections of Three Electronic States Affect the Ground State of Radical Species with Little or No Symmetry: A Pyrazolyl. Journal of the American Chemical Society, 2003, 125, 12428-12429.	13.7	47
105	Beyond Two-State Conical Intersections. Three-State Conical Intersections in Low Symmetry Molecules: the Allyl Radical. Journal of the American Chemical Society, 2003, 125, 10672-10676.	13.7	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 H ₂ O+O(3P) $\hat{\rightarrow}$ OH(A $\hat{\leftarrow}$ S ₂ $\hat{\leftarrow}$)+OH(X $\hat{\leftarrow}$ S ₂ $\hat{\leftarrow}$). Journal of Chemical Physics, 2002, 117, 3733-3740.	3.0	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.	3.0	23

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109	Photodissociation of the vinyloxy radical through conical, and avoided, intersections. <i>Journal of Chemical Physics</i> , 2002, 117, 7198-7206.	3.0	23
110	Spin-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 Case. <i>Journal of Physical Chemistry B</i> , 2002, 106, 8108-8116.	2.6	18
111	Accidental conical intersections of three states of the same symmetry. I. Location and relevance. <i>Journal of Chemical Physics</i> , 2002, 117, 6907-6910.	3.0	68
112	Intersecting Conical Intersection Seams: Their Location, Representation, and Effect on Local Topography. <i>Journal of Physical Chemistry A</i> , 2002, 106, 2580-2591.	2.5	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. <i>Journal of Chemical Physics</i> , 2001, 115, 2038-2050.	3.0	28
114	Actinyl Ions in Cs ₂ UO ₂ Cl ₄ . <i>Journal of Physical Chemistry A</i> , 2001, 105, 637-645.	2.5	86
115	On the effects of spin-orbit coupling on conical intersection seams in molecules with an odd number of electrons. II. Characterizing the local topography of the seam. <i>Journal of Chemical Physics</i> , 2001, 115, 5066-5075.	3.0	20
116	Intensities in the Spectra of Actinyl Ions. <i>Journal of Physical Chemistry A</i> , 2000, 104, 11983-11992.	2.5	68
117	Electronic Spectrum of the NpO ₂ ²⁺ and NpO ₂ ⁺ Ions. <i>Journal of Physical Chemistry A</i> , 2000, 104, 4064-4068.	2.5	87
118	Spin-Orbit Splittings in Mg ⁺ Neutral Complexes. <i>Journal of Physical Chemistry A</i> , 1998, 102, 1652-1656.	2.5	20
119	Projected Complex Absorbing Potential Multireference Configuration Interaction Approach for Shape and Feshbach Resonances. <i>Journal of Chemical Theory and Computation</i> , 0, , .	5.3	7