Michael Bearpark

List of Publications by Year
in descending order

101 papers	4,307 citations	87888 38 h-index	114465 63 g-index
104 all docs	104 docs citations	104 times ranked	3093 citing authors

#	Article	IF	Citations
1	A direct method for the location of the lowest energy point on a potential surface crossing. Chemical Physics Letters, 1994, 223, 269-274.	2.6	639
2	Can Diarylethene Photochromism Be Explained by a Reaction Path Alone? A CASSCF Study with Model MMVB Dynamics. Journal of Physical Chemistry A, 2003, 107, 11139-11152.	2.5	166
3	The Azulene S1State Decays via a Conical Intersection:Â A CASSCF Study with MMVB Dynamics. Journal of the American Chemical Society, 1996, 118, 169-175.	13.7	163
4	Relaxation Paths from a Conical Intersection:Â The Mechanism of Product Formation in the Cyclohexadiene/Hexatriene Photochemical Interconversion. Journal of Physical Chemistry A, 1997, 101, 2023-2032.	2.5	149
5	Electron Dynamics upon Ionization of Polyatomic Molecules: Coupling to Quantum Nuclear Motion and Decoherence. Physical Review Letters, 2017, 118, 083001.	7.8	133
6	â€˜Classical wavepacketâ€™ dynamics through a conical intersection. Application to the S1/S0 photochemistry of benzene. Chemical Physics Letters, 1995, 242, 27-32.	2.6	107
7	New Algorithms for Optimizing and Linking Conical Intersection Points. Journal of Chemical Theory and Computation, 2008, 4, 257-266.	5.3	97
8	Cooperating Rings incis-Stilbene Lead to an S0/S1Conical Intersection. Journal of Physical Chemistry A, 1997, 101, 3841-3847.	2.5	94
9	Can Fulvene S1Decay Be Controlled? A CASSCF Study with MMVB Dynamics. Journal of the American Chemical Society, 1996, 118, 5254-5260.	13.7	89
10	A computational strategy for geometry optimization of ionic and covalent excited states, applied to butadiene and hexatriene. Journal of Chemical Physics, 2004, 120, 7849-7860.	3.0	72
11	Molecular mechanics valence bond methods for large active spaces. Application to conjugated polycyclic hydrocarbons. Chemical Physics Letters, 1994, 217, 513-519.	2.6	71
12	Quadratic Description of Conical Intersections:â€‰ Characterization of Critical Points on the Extended Seam. Journal of Physical Chemistry A, 2007, 111, 2182-2192.	2.5	70
13	Electron dynamics following photoionization: Decoherence due to the nuclear-wave-packet width. Physical Review A, 2015, 92, .	2.5	70
14	Dihydroazulene/Vinylheptafulvene Photochromism:Â A Model for One-Way Photochemistry via a Conical Intersection. Journal of the American Chemical Society, 2002, 124, 1456-1470.	13.7	67
15	Conical intersections: A perspective on the computation of spectroscopic Jahnâ€“Teller parameters and the degenerate â€˜intersection spaceâ€™. Physical Chemistry Chemical Physics, 2005, 7, 2100.	2.8	67
16	Excitedâ€State Decay in the Photoisomerisation of Azobenzene: A New Balance between Mechanisms. ChemPhysChem, 2016, 17, 3068-3079.	2.1	66
17	Coupled electron-nuclear dynamics: Charge migration and charge transfer initiated near a conical intersection. Journal of Chemical Physics, 2013, 139, 044110.	3.0	65
18	Non-adiabatic dynamics close to conical intersections and the surface hopping perspective. Frontiers in Chemistry, 2014, 2, 97.	3.6	64

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19	Controlling S₁/S₀ Decay and the Balance between Photochemistry and Photostability in Benzene: A Direct Quantum Dynamics Study. Journal of Physical Chemistry A, 2008, 112, 13017-13027.	2.5	60
20	Significance of a Zwitterionic State for Fulgide Photochromism: Implications for the Design of Mimics. Angewandte Chemie - International Edition, 2010, 49, 2913-2916.	13.8	58
21	The response of the electronic structure to electronic excitation and double bond torsion in fulvene: a combined QTAIM, stress tensor and MO perspective. Physical Chemistry Chemical Physics, 2014, 16, 7115-7126.	2.8	58
22	The curvature of the conical intersection seam: An approximate second-order analysis. Journal of Chemical Physics, 2004, 121, 11562-11571.	3.0	57
23	Mixed state `on the fly' non-adiabatic dynamics: the role of the conical intersection topology. Chemical Physics Letters, 1998, 292, 259-266.	2.6	55
24	The First Structurally Characterized Hypervalent Silicon Hydride:Â Unexpected Molecular Geometry and Siâ^'HÂ·Â·Â·K Interactions. Journal of the American Chemical Society, 2001, 123, 7736-7737.	13.7	55
25	CASSCF calculations for photoinduced processes in large molecules: Choosing when to use the RASSCF, ONIOM and MMVB approximations. Journal of Photochemistry and Photobiology A: Chemistry, 2007, 190, 207-227.	3.9	55
26	An analytical second-order description of the S 0 /S 1 intersection seam: fulvene revisited. Theoretical Chemistry Accounts, 2007, 118, 241-251.	1.4	53
27	Conical Intersection Pathways in the Photocycloaddition of Ethene and Benzene:Â A CASSCF Study with MMVB Dynamics. Journal of the American Chemical Society, 1996, 118, 7353-7360.	13.7	50
28	Product Distribution in the Photolysis of s-cis Butadiene:Â A Dynamics Simulation. Journal of Physical Chemistry A, 2001, 105, 11496-11504.	2.5	50
29	Controlling the mechanism of fulvene S1/S0 decay: switching off the stepwise population transfer. Physical Chemistry Chemical Physics, 2010, 12, 15725.	2.8	50
30	Towards converging non-adiabatic direct dynamics calculations using frozen-width variational Gaussian product basis functions. Journal of Chemical Physics, 2012, 137, 22A548.	3.0	50
31	Toward a Mechanistic Understanding of the Photochromism of Dimethyldihydropyrenes. Journal of Organic Chemistry, 2007, 72, 4497-4503.	3.2	47
32	Relaxation Paths and Dynamics of Photoexcited Polyene Chains:Â Evidence for Creation and Annihilation of Neutral Soliton Pairs. Journal of the American Chemical Society, 2000, 122, 5568-5581.	13.7	46
33	Searching for Conical Intersections of Potential Energy Surfaces with the ONIOM Method: Application to Previtamin D. Journal of Physical Chemistry A, 2008, 112, 7286-7295.	2.5	45
34	The pseudo-Jahnâ€"Teller effect: a CASSCF diagnostic. Molecular Physics, 2002, 100, 1735-1739.	1.7	43
35	The second-order Ehrenfest method. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	42
36	Photostability Via Sloped Conical Intersections:â€‰ A Computational Study of the Excited States of the Naphthalene Radical Cation. Journal of Physical Chemistry A, 2006, 110, 13591-13599.	2.5	40

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37	Automatic generation of active coordinates for quantum dynamics calculations: Application to the dynamics of benzene photochemistry. Journal of Chemical Physics, 2008, 128, 124307.	3.0	39
38	Direct methods for non-adiabatic dynamics: connecting the single-set variational multi-configuration Gaussian (vMCG) and Ehrenfest perspectives. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	39
39	Mechanism of the Oxadi-Ï€-methane and [1,3]-Acyl Sigmatropic Rearrangements of Î²,Î³-Enones:Â A Theoretical Study. Journal of the American Chemical Society, 1996, 118, 176-184.	13.7	38
40	A valence-bond-based complete-active-space self-consistent-field method for the evaluation of bonding in organic molecules. Theoretical Chemistry Accounts, 2003, 110, 92-99.	1.4	38
41	Excited States of Conjugated Hydrocarbons Using the Molecular Mechanics - Valence Bond (MMVB) Method: Conical Intersections and Dynamics. Theoretical Chemistry Accounts, 2006, 116, 670-682.	1.4	36
42	New insights into the by-product fatigue mechanism of the photo-induced ring-opening in diarylethenes. Physical Chemistry Chemical Physics, 2014, 16, 18463-18471.	2.8	36
43	Electron dynamics upon ionization: Control of the timescale through chemical substitution and effect of nuclear motion. Journal of Chemical Physics, 2015, 142, 094105.	3.0	36
44	Benchmarking the Molecular Mechanicsâ^'Valence Bond Method:â€‰ Photophysics of Styrene and Indene. Journal of Physical Chemistry A, 1997, 101, 8395-8401.	2.5	34
45	Communication: Oscillating charge migration between lone pairs persists without significant interaction with nuclear motion in the glycine and Gly-Gly-NH-CH3 radical cations. Journal of Chemical Physics, 2014, 140, 201102.	3.0	33
46	A simple approach for improving the hybrid MMVB force field: Application to the photoisomerization ofs-cis butadiene. Journal of Computational Chemistry, 2003, 24, 1357-1363.	3.3	30
47	Ring puckering of cyclooctatetraene and cyclohexane is induced by pseudo-Jahnâ€“Teller coupling. Molecular Physics, 2006, 104, 2007-2010.	1.7	29
48	Electronic Control of Initial Nuclear Dynamics Adjacent to a Conical Intersection. Journal of Physical Chemistry A, 2015, 119, 5165-5172.	2.5	29
49	Photostability via Sloped Conical Intersections: A Computational Study of the Pyrene Radical Cation. Journal of Physical Chemistry A, 2008, 112, 10881-10886.	2.5	28
50	How the Conical Intersection Seam Controls Chemical Selectivity in the Photocycloaddition of Ethylene and Benzene. Journal of Organic Chemistry, 2013, 78, 1874-1886.	3.2	28
51	Mapping the intersection space of the ground and first excited states of fulvene. Molecular Physics, 2006, 104, 1033-1038.	1.7	27
52	Electron and nuclear dynamics following ionisation of modified bismethylene-adamantane. Faraday Discussions, 2016, 194, 95-115.	3.2	26
53	Characterization of the indacene S0/S1 conical intersection: An MMVB and CASSCF study. Molecular Physics, 1999, 96, 645-652.	1.7	25
54	Nuclear spatial delocalization silences electron density oscillations in 2-phenyl-ethyl-amine (PEA) and 2-phenylethyl-N,N-dimethylamine (PENNA) cations. Journal of Chemical Physics, 2016, 144, 104110.	3.0	25

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55	Analytical Harmonic Vibrational Frequencies for the Green Fluorescent Protein Computed with ONIOM: Chromophore Mode Character and Its Response to Environment. Journal of Chemical Theory and Computation, 2014, 10, 751-766.	5.3	24
56	Charge migration in polycyclic norbornadiene cations: Winning the race against decoherence. Journal of Chemical Physics, 2016, 145, 164103.	3.0	24
57	Modeling multidimensional spectral lineshapes from first principles: application to water-solvated adenine. Faraday Discussions, 2019, 221, 219-244.	3.2	24
58	Potential energy surfaces of pseudoaromatic molecules: An MMVB and CASSCF study of pentalene. International Journal of Quantum Chemistry, 1996, 60, 505-512.	2.0	23
59	Hydrogen bonds between ammonium ions and aromatic rings exist and have key consequences on solid-state and solution phase properties. New Journal of Chemistry, 2005, 29, 64.	2.8	23
60	Photostability via a Sloped Conical Intersection:Â A CASSCF and RASSCF Study of Pyracylene. Journal of Physical Chemistry A, 2005, 109, 8849-8856.	2.5	22
61	Photochemical Reactivity of 2-Vinylbiphenyl and 2-Vinyl-1,3-terphenyl:Â The Balance between Nonadiabatic and Adiabatic Photocyclization. Journal of the American Chemical Society, 2006, 128, 10533-10540.	13.7	22
62	Fluorescence of the perylene radical cation and an inaccessible D/D1 conical intersection: An MMVB, RASSCF, and TD-DFT computational study. Journal of Chemical Physics, 2010, 132, 044306.	3.0	22
63	Choosing RASSCF orbital active spaces for multiple electronic states. Computational and Theoretical Chemistry, 2014, 1040-1041, 14-19.	2.5	22
64	Competition between photodetachment and autodetachment of the $m {2^1pi pi ^*}$21Ï€Ï€* state of the green fluorescent protein chromophore anion. Journal of Chemical Physics, 2014, 140, 205103.	3.0	21
65	A Three-State Nonadiabatic Model for Intramolecular Electronic Energy Transfer (IEET) in 9-Anthryl-1â€˜-naphthylalkanes Studied by Molecular Mechanics/Valence Bond Dynamics. Journal of the American Chemical Society, 2000, 122, 5801-5810.	13.7	20
66	Bulk ferromagnetism in nitronyl nitroxide crystals: a first principles bottom-up comparative study of four bulk nitronyl nitroxide ferromagnets (KAXHAS, YOMYII, LICMIT and YUJNEW). Molecular Physics, 2006, 104, 857-873.	1.7	20
67	Ultrafast and radiationless electronic excited state decay of uracil and thymine cations: computing the effects of dynamic electron correlation. Physical Chemistry Chemical Physics, 2019, 21, 14322-14330.	2.8	19
68	Minimising biases in full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2015, 142, 104101.	3.0	18
69	Molecular mechanics-valence bond method for planar conjugated hydrocarbon cations. Journal of Chemical Physics, 2007, 127, 134111.	3.0	17
70	Charge migration engineered by localisation: electron-nuclear dynamics in polyenes and glycine. Molecular Physics, 2018, 116, 2474-2489.	1.7	16
71	Excited states of conjugated hydrocarbon radicals using the molecular mechanics ? valence bond (MMVB) method. Theoretical Chemistry Accounts, 2003, 110, 105-114.	1.4	15
72	Product Distributions from Molecular Mechanicsâ^'Valence Bond Dynamics:Â Modeling Photochemical [4 + 4] Cycloadditions. Journal of Organic Chemistry, 1998, 63, 4594-4600.	3.2	14

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73	Modeling the Photophysics and Photochromic Potential of 1,2-Dihydronaphthalene (DHN): A Combined CASPT2//CASSCF-Topological and MMVB-Dynamical Investigation. Journal of Physical Chemistry A, 2008, 112, 10096-10107.	2.5	14
74	The extended S₁/S₀ conical intersection seam for the photochemical 2â€‰+â€‰2 cycloaddition of two ethylene molecules. Molecular Physics, 2012, 110, 2493-2501.	1.7	14
75	Geometric Rotation of the Nuclear Gradient at a Conical Intersection: Extension to Complex Rotation of Diabatic States. Journal of Chemical Theory and Computation, 2015, 11, 3115-3122.	5.3	14
76	The unusual solid state structure of heroin hydrochloride monohydrate and its selective detection using NQR spectroscopy. New Journal of Chemistry, 2004, 28, 1309.	2.8	13
77	Photochemical reaction paths of cis-dienes studied with RASSCF: the changing balance between ionic and covalent excited states. Molecular Physics, 2015, 113, 1978-1990.	1.7	13
78	[18]Annulene: a benzene-like S0/S1 conical intersection located with CASSCF + GVB. Molecular Physics, 1996, 89, 37-46.	1.7	12
79	Understanding and improving the efficiency of full configuration interaction quantum Monte Carlo. Journal of Chemical Physics, 2016, 144, 094110.	3.0	12
80	Computing the Ultrafast and Radiationless Electronic Excited State Decay of Cytosine and 5â€methylâ€cytosine Cations: Uncovering the Role of Dynamic Electron Correlation. ChemPhotoChem, 2019, 3, 856-865.	3.0	12
81	Deconstructing the ONIOM Hessian: Investigating Method Combinations for Transition Structures. Journal of Chemical Theory and Computation, 2012, 8, 4907-4914.	5.3	10
82	Molecular excited state calculations with adaptive wavefunctions on a quantum eigensolver emulation: reducing circuit depth and separating spin states. Physical Chemistry Chemical Physics, 2021, 23, 26438-26450.	2.8	10
83	Conical Intersection Species as Reactive Intermediates. , 0, , 379-414.		8
84	Molecular Vertical Excitation Energies Studied with First-Order RASSCF (RAS[1,1]): Balancing Covalent and Ionic Excited States. Journal of Physical Chemistry A, 2019, 123, 5223-5230.	2.5	7
85	Second-Order Analysis of Conical Intersections: Applications to Photochemistry and Photophysics of Organic Molecules. Springer Series in Chemical Physics, 2009, , 169-200.	0.2	7
86	Comment on â€œFluorescence of Antiaromatic Systems:â€‰ An Experimental and Theoretical Study of 1,3,5-Tri-tert-butylpentaleneâ€. Journal of Physical Chemistry A, 2000, 104, 1075-1077.	2.5	6
87	Using Density Functional Theory Based Methods to Investigate the Photophysics of Polycyclic Aromatic Hydrocarbon Radical Cations: A Benchmark Study on Naphthalene, Pyrene and Perylene Cations. ChemPhotoChem, 2019, 3, 763-769.	3.0	6
88	A computational study of the Dougherty model for the prediction of high-spin states in organic chemistry. Theoretical Chemistry Accounts, 1999, 102, 309-316.	1.4	5
89	Application of the unitary group approach to evaluate spin density for configuration interaction calculations in a basis of S² eigenfunctions. International Journal of Quantum Chemistry, 2018, 118, e25559.	2.0	5
90	Radical-Triggered Reaction Mechanism of the Green-to-Red Photoconversion of EosFP. Journal of Physical Chemistry B, 2020, 124, 7765-7778.	2.6	5

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91	Modelling Photoionisation in Isocytosine: Potential Formation of Longerâ€Lived Excited State Cations in its Keto Form. ChemPhysChem, 2021, 22, 2172-2181.	2.1	5
92	Modelling Photoionisations in Tautomeric DNA Nucleobase Derivatives 7H-Adenine and 7H-Guanine: Ultrafast Decay and Photostability. Photochem, 2021, 1, 287-301.	2.2	4
93	CHAMP is a HPC Access and Metadata Portal. Journal of Open Source Software, 2022, 7, 3824.	4.6	4
94	Theoretical Modelling as a Possible Tool in the Design of Photochromic Systems. Molecular Crystals and Liquid Crystals, 2000, 344, 31-39.	0.3	3
95	Interpreting the excited states and decay processes of bichromophoric 1-phenyl-1,3-butadiene using CASSCF calculations. Molecular Physics, 2006, 104, 1017-1032.	1.7	3
96	CASSCF Calculations for Excited States of Large Molecules: Choosing when to use the RASSCF, ONIOM and MMVB Approximations. AIP Conference Proceedings, 2007, , .	0.4	3
97	How electronic superpositions drive nuclear motion following the creation of a localized hole in the glycine radical cation. Journal of Chemical Physics, 0, , .	3.0	3
98	The role of extended conical intersection seams in photochromic systems. , 2015, , .		1
99	Modelling Photoionisation in Isocytosine: Potential Formation of Longerâ€Lived Excited State Cations in its Keto Form. ChemPhysChem, 2021, 22, 2140-2140.	2.1	1
100	Three-layer ONIOM Studies of Rhodopsin in the Dark State: Shedding Light on the Protonation State of Glu-181. AIP Conference Proceedings, 2007, , .	0.4	0
101	10.1063/1.4943273.1. , 2016, , .		0