

# Martin J Paterson

## List of Publications by Year in descending order

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118  
papers

4,062  
citations

101384

36  
h-index

133063

59  
g-index

120  
all docs

120  
docs citations

120  
times ranked

4941  
citing authors

#	ARTICLE	IF	CITATIONS
1	Targeted photoredox catalysis in cancer cells. <i>Nature Chemistry</i> , 2019, 11, 1041-1048.	6.6	293
2	Two-Photon Absorption in Tetraphenylporphycenes: Are Porphycenes Better Candidates than Porphyrins for Providing Optimal Optical Properties for Two-Photon Photodynamic Therapy?. <i>Journal of the American Chemical Society</i> , 2007, 129, 5188-5199.	6.6	189
3	A Conformationally Flexible, Urea-Based Tripodal Anion Receptor: Solid-State, Solution, and Theoretical Studies. <i>Journal of Organic Chemistry</i> , 2006, 71, 1598-1608.	1.7	155
4	Benchmarking two-photon absorption with CC3 quadratic response theory, and comparison with density-functional response theory. <i>Journal of Chemical Physics</i> , 2006, 124, 054322.	1.2	137
5	Theoretical Study of Benzotriazole UV Photostability: Ultrafast Deactivation through Coupled Proton and Electron Transfer Triggered by a Charge-Transfer State. <i>Journal of the American Chemical Society</i> , 2004, 126, 2912-2922.	6.6	132
6	Metformin selectively targets redox control of complex I energy transduction. <i>Redox Biology</i> , 2018, 14, 187-197.	3.9	115
7	Mechanism of an Exceptional Class of Photostabilizers: A Seam of Conical Intersection Parallel to Excited State Intramolecular Proton Transfer (ESIPT) in <i>o</i> -Hydroxyphenyl-(1,3,5)-triazine. <i>Journal of Physical Chemistry A</i> , 2005, 109, 7527-7537.	1.1	111
8	Structure Calculation of an Elastic Hydrogel from Sonication of Rigid Small Molecule Components. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 1058-1062.	7.2	107
9	Overview of Theoretical and Computational Methods Applied to the Oxygen-Organic Molecule Photosystem. <i>Photochemistry and Photobiology</i> , 2006, 82, 1136.	1.3	104
10	Organoiridium Photosensitizers Induce Specific Oxidative Attack on Proteins within Cancer Cells. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 14898-14902.	7.2	101
11	Time-resolved photoelectron imaging of excited state relaxation dynamics in phenol, catechol, resorcinol, and hydroquinone. <i>Journal of Chemical Physics</i> , 2012, 137, 184304.	1.2	96
12	Unraveling Ultrafast Dynamics in Photoexcited Aniline. <i>Journal of the American Chemical Society</i> , 2012, 134, 12578-12589.	6.6	80
13	Magnetism in metal-organic capsules. <i>Chemical Communications</i> , 2010, 46, 3484.	2.2	73
14	Non-Adiabatic Direct Dynamics Study of Chromium Hexacarbonyl Photodissociation. <i>Journal of Physical Chemistry A</i> , 2002, 106, 10494-10504.	1.1	70
15	Induced Fit Interanion Discrimination by Binding-Induced Excimer Formation. <i>Journal of the American Chemical Society</i> , 2008, 130, 4105-4113.	6.6	70
16	Polymer-Supported Photosensitizers for Oxidative Organic Transformations in Flow and under Visible Light Irradiation. <i>ACS Catalysis</i> , 2017, 7, 4602-4612.	5.5	70
17	Conical intersections: A perspective on the computation of spectroscopic Jahn-Teller parameters and the degenerate intersection space <sup>TM</sup> . <i>Physical Chemistry Chemical Physics</i> , 2005, 7, 2100.	1.3	67
18	Exploring quantum phenomena and vibrational control in $\dot{\gamma}^*$ mediated photochemistry. <i>Chemical Science</i> , 2013, 4, 993-1001.	3.7	67

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19	Ultrafast photo-induced ligand solvolysis of cis-[Ru(bipyridine) <sub>2</sub> (nicotinamide)] <sup>2+</sup> : experimental and theoretical insight into its photoactivation mechanism. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 19141-19155.	1.3	65
20	One- and Two-Photon Photosensitized Singlet Oxygen Production: Characterization of Aromatic Ketones as Sensitizer Standards. <i>Journal of Physical Chemistry A</i> , 2007, 111, 5756-5767.	1.1	61
21	A global picture of the S1/S0 conical intersection seam of benzene. <i>Chemical Physics</i> , 2010, 377, 60-65.	0.9	61
22	Fluorescent "Twist" Sensing by Induced Anion Stabilisation of a Planar Chromophore. <i>Chemistry - A European Journal</i> , 2010, 16, 2714-2718.	1.7	58
23	The curvature of the conical intersection seam: An approximate second-order analysis. <i>Journal of Chemical Physics</i> , 2004, 121, 11562-11571.	1.2	57
24	Following the excited state relaxation dynamics of indole and 5-hydroxyindole using time-resolved photoelectron spectroscopy. <i>Journal of Chemical Physics</i> , 2011, 135, 194307.	1.2	57
25	Wavepacket dynamics study of Cr(CO) <sub>5</sub> after formation by photodissociation: relaxation through an (E <sub>g</sub> ) <sup>+</sup> Jahn-Teller conical intersection. <i>Molecular Physics</i> , 2006, 104, 1095-1105.	0.8	52
26	Linear response functions for a vibrational configuration interaction state. <i>Journal of Chemical Physics</i> , 2006, 125, 214309.	1.2	51
27	Manipulating dynamics with chemical structure: probing vibrationally-enhanced tunnelling in photoexcited catechol. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 6879.	1.3	48
28	Biomolecular Mode of Action of Metformin in Relation to Its Copper Binding Properties. <i>Biochemistry</i> , 2014, 53, 787-795.	1.2	46
29	Gelation Landscape Engineering Using a Multi-Reaction Supramolecular Hydrogelator System. <i>Journal of the American Chemical Society</i> , 2015, 137, 14236-14239.	6.6	46
30	Anion Binding and Luminescent Sensing using Cationic Ruthenium(II) Aminopyridine Complexes. <i>Chemistry - A European Journal</i> , 2008, 14, 7296-7305.	1.7	43
31	Effects of conjugation length and resonance enhancement on two-photon absorption in phenylenevinylene oligomers. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 1177-1191.	1.3	43
32	Two-Photon Activated Ligand Exchange in Platinum(II) Complexes. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 11263-11266.	7.2	42
33	Ultraviolet relaxation dynamics of aniline, <i>N,N</i> -dimethylaniline and 3,5-dimethylaniline at 250 nm. <i>Journal of Chemical Physics</i> , 2015, 142, 114309.	1.2	42
34	Optical Excitations in Star-Shaped Fluorene Molecules. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2913-2919.	1.1	40
35	A quinolinium-derived turn-off fluorescent anion sensor. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 1010.	1.5	39
36	Conformational control by "zipping-up" an anion-binding unimolecular capsule. <i>Chemical Communications</i> , 2008, , 1395.	2.2	36

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37	Two-photon absorption cross sections: An investigation of solvent effects. Theoretical studies on formaldehyde and water. <i>Journal of Chemical Physics</i> , 2006, 125, 184501.	1.2	35
38	Intramolecular binding site competition as a means of tuning the response of a colourimetric anion sensor. <i>New Journal of Chemistry</i> , 2008, 32, 786.	1.4	35
39	Time resolved velocity map imaging of H-atom elimination from photoexcited imidazole and its methyl substituted derivatives. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 10342.	1.3	35
40	General Force-Field Parametrization Scheme for Molecular Dynamics Simulations of Conjugated Materials in Solution. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 3813-3824.	2.3	35
41	The role of novel Rydberg-valence behaviour in the non-adiabatic dynamics of tertiary aliphatic amines. <i>Chemical Science</i> , 2016, 7, 1826-1839.	3.7	34
42	Effect of exciton self-trapping and molecular conformation on photophysical properties of oligofluorenes. <i>Journal of Chemical Physics</i> , 2009, 131, 154906.	1.2	33
43	Bis( $\eta$ -heterocyclic carbene) Dipalladium Complexes: Synthesis, Solid State Conformational Studies and Solution Behaviour. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 2835-2843.	1.0	32
44	A simple chemical model for clathrate hydrate inhibition by polyvinylcaprolactam. <i>Chemical Communications</i> , 2011, 47, 9891.	2.2	30
45	Photoinduced Electron Transfer in Squaraine Dyes: Sensitization of Large Band Gap Semiconductors. <i>Journal of Physical Chemistry A</i> , 2002, 106, 11431-11439.	1.1	29
46	Calculations of potential energy surfaces using Monte Carlo configuration interaction. <i>Journal of Chemical Physics</i> , 2012, 137, 194111.	1.2	29
47	Ultrafast relaxation dynamics of electronically excited piperidine: ionization signatures of Rydberg/valence evolution. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 25070-25079.	1.3	29
48	Mapping the intersection space of the ground and first excited states of fulvene. <i>Molecular Physics</i> , 2006, 104, 1033-1038.	0.8	27
49	Colourimetric Carboxylate Anion Sensors Derived from Viologen Based Receptors. <i>Chemistry - A European Journal</i> , 2010, 16, 1480-1492.	1.7	27
50	Calculations of the low-lying excited states of the TiO <sub>2</sub> molecule. <i>Journal of Chemical Physics</i> , 2010, 133, 204302.	1.2	26
51	Vibronic Coupling In Inorganic Systems: Photochemistry, Conical Intersections, And The Jahn-Teller And Pseudo-Jahn-Teller Effects. <i>Advances in Inorganic Chemistry</i> , 2010, , 351-390.	0.4	24
52	Enantioselective lactate binding by chiral tripodal anion hosts derived from amino acids. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 1554.	1.5	21
53	The structure and UV spectroscopy of benzene-water (Bz-W <sub>6</sub> ) clusters using time-dependent density functional theory. <i>Photochemical and Photobiological Sciences</i> , 2014, 13, 1549-1560.	1.6	20
54	Multireference X-ray emission and absorption spectroscopy calculations from Monte Carlo configuration interaction. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	20

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55	Comparing the ultraviolet photostability of azole chromophores. <i>Chemical Science</i> , 2012, 3, 1192.	3.7	19
56	Excited-State Absorption of Conjugated Polymers in the Near-Infrared and Visible: A Computational Study of Oligofluorenes. <i>Journal of Physical Chemistry C</i> , 2013, 117, 6889-6895.	1.5	19
57	Steric control of sorting regimes in self-assembled cages. <i>Chemical Communications</i> , 2021, 57, 12456-12459.	2.2	19
58	Monte Carlo configuration interaction applied to multipole moments, ionization energies, and electron affinities. <i>Journal of Computational Chemistry</i> , 2013, 34, 1083-1093.	1.5	18
59	Relaxation dynamics of photoexcited resorcinol: internal conversion versus H atom tunnelling. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 550-562.	1.3	18
60	Observation of multi-channel non-adiabatic dynamics in aniline derivatives using time-resolved photoelectron imaging. <i>Faraday Discussions</i> , 2016, 194, 185-208.	1.6	18
61	Transition Metal Complexes of Calix[4]arene: Theoretical Investigations into Small Guest Binding within the Host Cavity. <i>Journal of Physical Chemistry A</i> , 2016, 120, 824-839.	1.1	18
62	Template-free hierarchical self-assembly of a pyrene derivative into supramolecular nanorods. <i>Chemical Communications</i> , 2017, 53, 1973-1976.	2.2	18
63	DNA-Intercalative Platinum Anticancer Complexes Photoactivated by Visible Light. <i>Chemistry - A European Journal</i> , 2021, 27, 10711-10716.	1.7	18
64	Photoactivated Osmium Arene Anticancer Complexes. <i>Inorganic Chemistry</i> , 2021, 60, 17450-17461.	1.9	18
65	Two-Photon Absorption-Molecular Structure Investigation Using a Porphycene Chromophore with Potential in Photodynamic Therapy. <i>Journal of Physical Chemistry B</i> , 2012, 116, 11818-11828.	1.2	17
66	Vibronic coupling effects on the structure and spectroscopy of neutral and charged TiO <sub>2</sub> clusters. <i>Chemical Physics</i> , 2012, 408, 1-10.	0.9	16
67	Two-photon absorption in porphycenic macrocycles: the effect of tuning the core aromatic electronic structure. <i>Chemical Communications</i> , 2012, 48, 1544-1546.	2.2	16
68	Time-resolved photoionization spectroscopy of mixed Rydberg-valence states: indole case study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 26659-26669.	1.3	16
69	Halogenation effects in intramolecular furan Diels-Alder reactions: broad scope synthetic and computational studies. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 7946.	1.5	15
70	Excited electronic states of MnO <sub>4</sub> <sup>2-</sup> : Challenges for wavefunction and density functional response theories. <i>Chemical Physics</i> , 2015, 446, 86-91.	0.9	15
71	Organoiridium Photosensitizers Induce Specific Oxidative Attack on Proteins within Cancer Cells. <i>Angewandte Chemie</i> , 2017, 129, 15094-15098.	1.6	15
72	On the linear and non-linear electronic spectroscopy of chlorophylls: a computational study. <i>Photochemical and Photobiological Sciences</i> , 2014, 13, 103-111.	1.6	13

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73	Self-trapping and excited state absorption in fluorene homo-polymer and copolymers with benzothiadiazole and tri-phenylamine. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 21937-21948.	1.3	13
74	Excited states of porphyrin and porphycene aggregates: Computational insights. <i>Computational and Theoretical Chemistry</i> , 2014, 1040-1041, 274-286.	1.1	12
75	Theoretical Study of the Pseudo-Jahn-Teller Effect in the Edge-Sharing Bioctahedral Complex $\text{Mo}_2(\text{DXylF})_2(\text{O}_2\text{CCH}_3)_2(\text{H}_2\text{O})_2$ . <i>Inorganic Chemistry</i> , 2009, 48, 10652-10657.	1.9	11
76	Ground and excited states of naphthalene-water ( $\text{naphtha}_6$ ) clusters: a computational study. <i>RSC Advances</i> , 2015, 5, 28281-28291.	1.7	11
77	View from the bridge: a pseudo-Jahn-Teller approach to transition metal hydrosilane complexes. <i>New Journal of Chemistry</i> , 2004, 28, 1434-1436.	1.4	10
78	Photostereochemistry and Photoaquation Reactions of $[\text{Cr}(\text{tn})_3]^{3+}$ : Theoretical Studies Show the Importance of Reduced Coordination Conical Intersection Geometries. <i>Journal of Physical Chemistry A</i> , 2012, 116, 5375-5382.	1.1	10
79	Elucidating the Ring Inversion Mechanism(s) for Biscalixarenes. <i>Journal of Physical Chemistry A</i> , 2014, 118, 7986-8001.	1.1	10
80	Excited States of the Nickel Carbonyls $\text{Ni}(\text{CO})$ and $\text{Ni}(\text{CO})_4$ : Challenging Molecules for Electronic Structure Theory. <i>Journal of Physical Chemistry A</i> , 2015, 119, 10076-10083.	1.1	10
81	Intramolecular Nitrofuran Diels-Alder Reactions: Extremely Substituent-Tolerant Cycloadditions via Asynchronous Transition States. <i>Journal of Organic Chemistry</i> , 2017, 82, 6656-6670.	1.7	10
82	Stress Tensor Eigenvector Following with Next-Generation Quantum Theory of Atoms in Molecules: Excited State Photochemical Reaction Path from Benzene to Benzvalene. <i>Journal of Physical Chemistry A</i> , 2019, 123, 8254-8264.	1.1	10
83	One- and Two-Photon-Induced Photochemistry of Iron Pentacarbonyl $[\text{Fe}(\text{CO})_5]$ : Insights from Coupled Cluster Response Theory. <i>ChemPhotoChem</i> , 2019, 3, 825-832.	1.5	10
84	Rydberg-to-valence evolution in excited state molecular dynamics. <i>International Reviews in Physical Chemistry</i> , 2020, 39, 517-567.	0.9	10
85	Influence of electronic effects on one- and two-photon absorption in porphyrin isomers. <i>RSC Advances</i> , 2013, 3, 9247.	1.7	9
86	Crossed McMurry Coupling Reactions for Porphycenic Macrocycles: Non-Statistical Selectivity and Rationalisation. <i>European Journal of Organic Chemistry</i> , 2015, 2015, 3818-3823.	1.2	9
87	Bis-Calix[4]arenes: From Ligand Design to the Directed Assembly of a Metal-Organic Trigonal Antiprism. <i>Chemistry - A European Journal</i> , 2016, 22, 8791-8795.	1.7	9
88	Toward Understanding of the Lower Rim Binding Preferences of Calix[4]arene. <i>Journal of Physical Chemistry A</i> , 2015, 119, 5804-5815.	1.1	8
89	Control of chirality, bond flexing and anharmonicity in an electric field. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26793.	1.0	8
90	Ultraviolet Excitation Dynamics of Nitrobenzenes. <i>Journal of Physical Chemistry A</i> , 2021, 125, 7174-7184.	1.1	8

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91	Chirality without Stereoisomers: Insight from the Helical Response of Bond Electrons. <i>ChemPhysChem</i> , 2021, 22, 1989-1995.	1.0	8
92	A Simple Fluorescent Ion-Pair Binding Host that Acts as an "AND" Logic Gate. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 3879-3882.	1.0	7
93	Photoracemization and excited state relaxation through non-adiabatic pathways in chromium (III) oxalate ions. <i>Journal of Chemical Physics</i> , 2012, 137, 034308.	1.2	7
94	Computation of Excited States of Transition Metal Complexes. <i>Structure and Bonding</i> , 2014, , 107-138.	1.0	7
95	Vacuum ultraviolet excited state dynamics of small amides. <i>Journal of Chemical Physics</i> , 2019, 150, 054301.	1.2	7
96	Systematic Study of the Effect of Lower-Rim Methylation on Small Guest Binding within the Host Cavity of Calix[4]arene. <i>Journal of Physical Chemistry A</i> , 2017, 121, 7986-7992.	1.1	6
97	Targetable Mechanical Properties by Switching between Self-Sorting and Co-Assembly with <i>In Situ</i> Formed Tripodal Ketoenamine Supramolecular Hydrogels. <i>ChemNanoMat</i> , 2018, 4, 853-859.	1.5	6
98	The influence of substituent position on the excited state dynamics operating in 4-, 5- and 6-hydroxyindole. <i>Chemical Physics Letters</i> , 2020, 738, 136870.	1.2	6
99	Theoretical determination of two-photon absorption in biologically relevant pterin derivatives. <i>Photochemical and Photobiological Sciences</i> , 2020, 19, 1538-1547.	1.6	6
100	Discrete Ti <sup>IV</sup> O <sup>2+</sup> Ti Complexes: Visible-Light-Activated, Homogeneous Alternative to TiO <sub>2</sub> Photosensitisers. <i>Chemistry - A European Journal</i> , 2020, 26, 9486-9494.	1.7	6
101	Photoisomerization in a Platinum <sup>II</sup> Amido Pincer Complex: An Excited-State Reaction Pathway Controlled by Localized Ligand Photochemistry. <i>Journal of Physical Chemistry Letters</i> , 2010, 1, 1301-1306.	2.1	5
102	A Time-Dependent Density Functional Theory Study of the Structure and Electronic Spectroscopy of the Group 7 Mixed-Metal Carbonyls: MnTc(CO) <sub>10</sub> , MnRe(CO) <sub>10</sub> , and TcRe(CO) <sub>10</sub> . <i>Journal of Physical Chemistry A</i> , 2012, 116, 9295-9304.	1.1	5
103	Computational Study of the Interactions between Benzene and Crystalline Ice I <sub>h</sub> : Ground and Excited States. <i>ChemPhysChem</i> , 2016, 17, 4079-4089.	1.0	5
104	The role of the natural transition orbital density in the SO <sup>+</sup> AS1 and SO <sup>+</sup> AS2 transitions of fulvene with next generation QTAIM. <i>Chemical Physics Letters</i> , 2020, 751, 137556.	1.2	5
105	Molecular properties and excited state van der Waals potentials in the NO A <sup>2</sup> $\Sigma^+$ + O <sub>2</sub> X <sup>2</sup> $\Sigma^+$ collision complex. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 7983-7993.	1.3	5
106	Development of spin-orbit coupling for stochastic configuration interaction techniques. <i>Journal of Computational Chemistry</i> , 2018, 39, 319-327.	1.5	4
107	A systematic construction of configuration interaction wavefunctions in the complete CI space. <i>Journal of Chemical Physics</i> , 2019, 151, 164112.	1.2	4
108	The Jahn-Teller Effect in Binary Transition Metal Carbonyl Complexes. <i>Springer Series in Chemical Physics</i> , 2009, , 311-344.	0.2	4

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109	Next generation quantum theory of atoms in molecules for the design of emitters exhibiting thermally activated delayed fluorescence with laser irradiation. <i>Journal of Computational Chemistry</i> , 2022, 43, 206-214.	1.5	4
110	Unusual Structure-Energy Correlations in Intramolecular Diels-Alder Reaction Transition States. <i>Molecules</i> , 2014, 19, 15535-15545.	1.7	3
111	Excited-State Dynamics of a Two-Photon-Activatable Ruthenium Prodrug. <i>ChemPhysChem</i> , 2016, 17, 221-224.	1.0	3
112	Positronic molecule calculations using Monte Carlo configuration interaction. <i>Chemical Physics Letters</i> , 2016, 645, 106-111.	1.2	3
113	Investigation of challenging spin systems using Monte Carlo configuration interaction and the density matrix renormalization group. <i>Journal of Computational Chemistry</i> , 2017, 38, 2701-2712.	1.5	3
114	Properties of Conjugated Materials from Quantum Chemistry Coupled to Molecular Dynamics Generated Ensembles. <i>Journal of Physical Chemistry A</i> , 2020, 124, 10667-10677.	1.1	1
115	Innentitelbild: Organoiridium Photosensitizer Induce Specific Oxidative Attack on Proteins within Cancer Cells ( <i>Angew. Chem.</i> 47/2017). <i>Angewandte Chemie</i> , 2017, 129, 14968-14968.	1.6	0
116	Frontispiece: Discrete Ti <sup>IV</sup> -O <sup>2-</sup> -Ti Complexes: Visible-Light-Activated, Homogeneous Alternative to TiO <sub>2</sub> Photosensitizers. <i>Chemistry - A European Journal</i> , 2020, 26, .	1.7	0
117	Chemical functionality at the liquid surface of pure unsaturated fatty acids. <i>Environmental Science Atmospheres</i> , 0, , .	0.9	0
118	The effect of substituents and their positions on a series of disubstituted naphthalene bromide salts towards intermolecular interactions and crystal packing. <i>CrystEngComm</i> , 0, , .	1.3	0