Thomas J Penfold

List of Publications by Year
in descending order

122 papers	6,974 citations	66343 42 h-index	62596 80 g-index
130 all docs	130 docs citations	130 times ranked	6022 citing authors

#	Article	IF	Citations
1	Revealing the spinâ€“vibronic coupling mechanism of thermally activated delayed fluorescence. Nature Communications, 2016, 7, 13680.	12.8	694
2	Spin-Vibronic Mechanism for Intersystem Crossing. Chemical Reviews, 2018, 118, 6975-7025.	47.7	592
3	The Importance of Vibronic Coupling for Efficient Reverse Intersystem Crossing in Thermally Activated Delayed Fluorescence Molecules. ChemPhysChem, 2016, 17, 2956-2961.	2.1	558
4	Photophysics of thermally activated delayed fluorescence molecules. Methods and Applications in Fluorescence, 2017, 5, 012001.	2.3	394
5	The theory of thermally activated delayed fluorescence for organic light emitting diodes. Chemical Communications, 2018, 54, 3926-3935.	4.1	239
6	Regio- and conformational isomerization critical to design of efficient thermally-activated delayed fluorescence emitters. Nature Communications, 2017, 8, 14987.	12.8	235
7	On Predicting the Excited-State Properties of Thermally Activated Delayed Fluorescence Emitters. Journal of Physical Chemistry C, 2015, 119, 13535-13544.	3.1	163
8	Recent experimental and theoretical developments in time-resolved X-ray spectroscopies. Coordination Chemistry Reviews, 2014, 277-278, 44-68.	18.8	161
9	Triazatruxene: A Rigid Central Donor Unit for a Dâ€“A₃ Thermally Activated Delayed Fluorescence Material Exhibiting Subâ€Microsecond Reverse Intersystem Crossing and Unity Quantum Yield via Multiple Singletâ€“Triplet State Pairs. Advanced Science, 2018, 5, 1700989.	11.2	145
10	Inverting the Handedness of Circularly Polarized Luminescence from Light-Emitting Polymers Using Film Thickness. ACS Nano, 2019, 13, 8099-8105.	14.6	145
11	Nonadiabatic coupling reduces the activation energy in thermally activated delayed fluorescence. Physical Chemistry Chemical Physics, 2017, 19, 8428-8434.	2.8	134
12	Pathways to increase the dissymmetry in the interaction of chiral light and chiral molecules. Chemical Science, 2021, 12, 8589-8602.	7.4	127
13	The role of solid state solvation on the charge transfer state of a thermally activated delayed fluorescence emitter. Journal of Materials Chemistry C, 2017, 5, 11001-11009.	5.5	115
14	Solvent-Induced Luminescence Quenching: Static and Time-Resolved X-Ray Absorption Spectroscopy of a Copper(I) Phenanthroline Complex. Journal of Physical Chemistry A, 2013, 117, 4591-4601.	2.5	111
15	Competing ultrafast intersystem crossing and internal conversion in the â€œchannel 3â€•region of benzene. Physical Chemistry Chemical Physics, 2010, 12, 15607.	2.8	102
16	Mapping of the Photoinduced Electron Traps in TiO₂ by Picosecond Xâ€•ray Absorption Spectroscopy. Angewandte Chemie - International Edition, 2014, 53, 5858-5862.	13.8	92
17	Ultrafast dynamics of the S1 excited state of benzene. Chemical Physics Letters, 2009, 469, 43-47.	2.6	84
18	Revealing hole trapping in zinc oxide nanoparticles by time-resolved X-ray spectroscopy. Nature Communications, 2018, 9, 478.	12.8	84

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19	The contributions of molecular vibrations and higher triplet levels to the intersystem crossing mechanism in metal-free organic emitters. Journal of Materials Chemistry C, 2017, 5, 6269-6280.	5.5	83
20	Synthesis and luminescence modulation of pyrazine-based gold(<scp>iii</scp>) pincer complexes. Chemical Communications, 2015, 51, 16629-16632.	4.1	79
21	A Quantum Dynamics Study of the Ultrafast Relaxation in a Prototypical Cu(I)â€“Phenanthroline. Journal of Physical Chemistry A, 2014, 118, 9861-9869.	2.5	74
22	A femtosecond fluorescence study of vibrational relaxation and cooling dynamics of UV dyes. Physical Chemistry Chemical Physics, 2012, 14, 3513.	2.8	73
23	Probing the Transition from Hydrophilic to Hydrophobic Solvation with Atomic Scale Resolution. Journal of the American Chemical Society, 2011, 133, 12740-12748.	13.7	71
24	X-ray Absorption Spectroscopy of Ground and Excited Rheniumâ€“Carbonylâ€“Diimine Complexes: Evidence for a Two-Center Electron Transfer. Journal of Physical Chemistry A, 2013, 117, 361-369.	2.5	63
25	High-Efficiency Iron Photosensitizer Explained with Quantum Wavepacket Dynamics. Journal of Physical Chemistry Letters, 2016, 7, 2009-2014.	4.6	61
26	A Deep Neural Network for the Rapid Prediction of X-ray Absorption Spectra. Journal of Physical Chemistry A, 2020, 124, 4263-4270.	2.5	60
27	The influence of molecular conformation on the photophysics of organic room temperature phosphorescent luminophores. Journal of Materials Chemistry C, 2018, 6, 9238-9247.	5.5	59
28	The intersystem crossing of a cyclic (alkyl)(amino) carbene gold (<scp>i</scp>) complex. Journal of Chemical Physics, 2018, 149, 014304.	3.0	56
29	Tracking multiple components of a nuclear wavepacket in photoexcited Cu(I)-phenanthroline complex using ultrafast X-ray spectroscopy. Nature Communications, 2019, 10, 3606.	12.8	56
30	The intersystem crossing mechanism of an ultrapure blue organoboron emitter. Organic Electronics, 2018, 59, 45-48.	2.6	55
31	Ultrafast core-loss spectroscopy in four-dimensional electron microscopy. Structural Dynamics, 2015, 2, 024302.	2.3	54
32	Circularly Polarised Luminescence from Helically Chiral â€œConfusedâ€• N,N,O,Câ€Boronâ€Chelated Dipyrromethenes (BODIPYs). ChemPhotoChem, 2017, 1, 513-517.	3.0	54
33	The influence of molecular geometry on the efficiency of thermally activated delayed fluorescence. Journal of Materials Chemistry C, 2019, 7, 6672-6684.	5.5	53
34	The effect of molecular distortions on spinâ€“orbit coupling in simple hydrocarbons. Chemical Physics, 2010, 375, 58-66.	1.9	50
35	Photooxidation and photoaquation of iron hexacyanide in aqueous solution: A picosecond X-ray absorption study. Structural Dynamics, 2014, 1, 024901.	2.3	49
36	Understanding and Designing Thermally Activated Delayed Fluorescence Emitters: Beyond the Energy Gap Approximation. Chemical Record, 2020, 20, 831-856.	5.8	49

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37	Photophysics of a copper phenanthroline elucidated by trajectory and wavepacket-based quantum dynamics: a synergetic approach. Physical Chemistry Chemical Physics, 2017, 19, 19590-19600.	2.8	48
38	Derivation of spin-orbit couplings in collinear linear-response TDDFT: A rigorous formulation. Journal of Chemical Physics, 2014, 140, 144103.	3.0	47
39	Probing wavepacket dynamics using ultrafast x-ray spectroscopy. Journal of Physics B: Atomic, Molecular and Optical Physics, 2015, 48, 214001.	1.5	46
40	Theoretical Rationalization of the Emission Properties of Prototypical Cu(I)â€“Phenanthroline Complexes. Journal of Physical Chemistry A, 2015, 119, 7026-7037.	2.5	45
41	Progress in the Theory of X-ray Spectroscopy: From Quantum Chemistry to Machine Learning and Ultrafast Dynamics. Journal of Physical Chemistry A, 2021, 125, 4276-4293.	2.5	44
42	The role of Hartreeâ€“Fock exchange in the simulation of X-ray absorption spectra: A study of photoexcited. Chemical Physics Letters, 2013, 580, 179-184.	2.6	43
43	Establishing nonlinearity thresholds with ultraintense X-ray pulses. Scientific Reports, 2016, 6, 33292.	3.3	43
44	Photoaquation Mechanism of Hexacyanoferrate(II) Ions: Ultrafast 2D UV and Transient Visible and IR Spectroscopies. Journal of the American Chemical Society, 2017, 139, 7335-7347.	13.7	43
45	Luminescent Gold(III) Thiolates: Supramolecular Interactions Trigger and Control Switchable Photoemissions from Bimolecular Excited States. Chemistry - A European Journal, 2017, 23, 105-113.	3.3	43
46	X-ray Spectroscopic Study of Solvent Effects on the Ferrous and Ferric Hexacyanide Anions. Journal of Physical Chemistry A, 2014, 118, 9411-9418.	2.5	42
47	Competition between the heavy atom effect and vibronic coupling in donorâ€“bridgeâ€“acceptor organometallics. Physical Chemistry Chemical Physics, 2020, 22, 4659-4667.	2.8	41
48	Probing the electronic and geometric structure of ferric and ferrous myoglobins in physiological solutions by Fe K-edge absorption spectroscopy. Physical Chemistry Chemical Physics, 2014, 16, 1617-1631.	2.8	39
49	A wavelet analysis for the X-ray absorption spectra of molecules. Journal of Chemical Physics, 2013, 138, 014104.	3.0	38
50	Quantum dynamics study of the competing ultrafast intersystem crossing and internal conversion in the â€œchannel 3â€•region of benzene. Journal of Chemical Physics, 2012, 137, 204310.	3.0	37
51	Effect of tert-Butyl Functionalization on the Photoexcited Decay of a Fe(II)-N-Heterocyclic Carbene Complex. Journal of Physical Chemistry C, 2016, 120, 17234-17241.	3.1	37
52	Influence of Heavy Atom Effect on the Photophysics of Coinage Metal Carbeneâ€Metalâ€Amide Emitters. Advanced Functional Materials, 2021, 31, 2005438.	14.9	37
53	Exceptionally fast radiative decay of a dinuclear platinum complex through thermally activated delayed fluorescence. Chemical Science, 2021, 12, 6172-6180.	7.4	37
54	A Vibronic Coupling Hamiltonian to Describe the Ultrafast Excited State Dynamics of a Cu(I)-Phenanthroline Complex. Chimia, 2014, 68, 227.	0.6	35

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55	A model Hamiltonian to simulate the complex photochemistry of benzene II. Journal of Chemical Physics, 2009, 131, 064303.	3.0	34
56	Ultrafast nonadiabatic dynamics probed by nitrogen K-edge absorption spectroscopy. Physical Chemistry Chemical Physics, 2020, 22, 2667-2676.	2.8	34
57	Using the Mechanical Bond to Tune the Performance of a Thermally Activated Delayed Fluorescence Emitter**. Angewandte Chemie - International Edition, 2021, 60, 12066-12073.	13.8	32
58	Open questions on the photophysics of thermally activated delayed fluorescence. Communications Chemistry, 2021, 4, .	4.5	32
59	NO binding kinetics in myoglobin investigated by picosecond Fe K-edge absorption spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 12922-12927.	7.1	30
60	Femtosecond X-ray emission study of the spin cross-over dynamics in haem proteins. Nature Communications, 2020, 11, 4145.	12.8	29
61	Evidence for a Peierls phase-transition in a three-dimensional multiple charge-density waves solid. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 5603-5608.	7.1	28
62	1,2,4-Triazines in the Synthesis of Bipyridine Bisphenolate ONNO Ligands and Their Highly Luminescent Tetradentate Pt(II) Complexes for Solution-Processable OLEDs. Inorganic Chemistry, 2018, 57, 3825-3832.	4.0	28
63	Hydrostatic Pressureâ€€controlled Ratiometric Luminescence Responses of a Dibenzo[a,j]phenazineâ€€cored Mechanoluminophore. ChemPhotoChem, 2019, 3, 1203-1211.	3.0	27
64	Local control of multidimensional dynamics. Physical Chemistry Chemical Physics, 2010, 12, 15616.	2.8	26
65	Simulations of X-ray absorption spectra: the effect of the solvent. Physical Chemistry Chemical Physics, 2012, 14, 9444.	2.8	25
66	Investigating interfacial electron transfer in dye-sensitized NiO using vibrational spectroscopy. Physical Chemistry Chemical Physics, 2017, 19, 7877-7885.	2.8	23
67	Pushing the Frontiers of First-Principles Based Computer Simulations of Chemical and Biological Systems. Chimia, 2011, 65, 667.	0.6	22
68	Local control theory in trajectory-based nonadiabatic dynamics. Physical Review A, 2011, 84, .	2.5	22
69	Characterizing the Structure and Defect Concentration of ZnO Nanoparticles in a Colloidal Solution. Journal of Physical Chemistry C, 2014, 118, 19422-19430.	3.1	22
70	Dâ€“A₃ TADF emitters: the role of the density of states for achieving faster triplet harvesting rates. Journal of Materials Chemistry C, 2019, 7, 12942-12952.	5.5	22
71	A quantum dynamics study of the hyperfluorescence mechanism. Journal of Materials Chemistry C, 2021, 9, 1362-1369.	5.5	21
72	Probing spinâ€“vibronic dynamics using femtosecond X-ray spectroscopy. Faraday Discussions, 2016, 194, 731-746.	3.2	20

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73	Excited State Intramolecular Proton Transfer Dynamics for Triplet Harvesting in Organic Molecules. Journal of Physical Chemistry A, 2019, 123, 2640-2649.	2.5	20
74	Structural Diversity and Argentophilic Interactions in One-Dimensional Silver-Based Coordination Polymers. Crystal Growth and Design, 2017, 17, 5753-5763.	3.0	19
75	Simulation of ultrafast excited-state dynamics and elastic x-ray scattering by quantum wavepacket dynamics. Journal of Chemical Physics, 2019, 151, 104307.	3.0	19
76	On the geometry dependence of tunedâ€range separated hybrid functionals. Journal of Computational Chemistry, 2019, 40, 2191-2199.	3.3	19
77	Non-equilibrium x-ray spectroscopy using direct quantum dynamics. Journal of Chemical Physics, 2018, 149, 124107.	3.0	18
78	Understanding the potential for efficient triplet harvesting with hot excitons. Faraday Discussions, 2019, 216, 395-413.	3.2	17
79	Accurate, affordable, and generalizable machine learning simulations of transition metal x-ray absorption spectra using the XANESNET deep neural network. Journal of Chemical Physics, 2022, 156, 164102.	3.0	17
80	Investigating DNA Radiation Damage Using X-Ray Absorption Spectroscopy. Biophysical Journal, 2016, 110, 1304-1311.	0.5	16
81	A monomeric methyllithium complex: synthesis and structure. Chemical Communications, 2021, 57, 6205-6208.	4.1	16
82	Identifying the major intermediate species by combining time-resolved X-ray solution scattering and X-ray absorption spectroscopy. Physical Chemistry Chemical Physics, 2015, 17, 23298-23302.	2.8	15
83	How To Excite Nuclear Wavepackets into Electronically Degenerate States in Spin-Vibronic Quantum Dynamics Simulations. Journal of Chemical Theory and Computation, 2018, 14, 3967-3974.	5.3	15
84	Redox Potentials of Polyoxometalates from an Implicit Solvent Model and QM/MM Molecular Dynamics. Journal of Physical Chemistry C, 2020, 124, 15045-15056.	3.1	13
85	The Role of Structural Representation in the Performance of a Deep Neural Network for X-ray Spectroscopy. Molecules, 2020, 25, 2715.	3.8	13
86	Hydrostatic Pressure-Induced Spectral Variation of Reichardtâ€™s Dye: A Polarity/Pressure Dual Indicator. ACS Omega, 2020, 5, 897-903.	3.5	13
87	On the factors influencing the chiroptical response of conjugated polymer thin films. Chemical Communications, 2021, 57, 9914-9917.	4.1	13
88	Excited state dynamics initiated by an electromagnetic field within the Variational Multi-Configurational Gaussian (vMCG) method. Computational and Theoretical Chemistry, 2019, 1160, 24-30.	2.5	12
89	Rapid predictions of the colour purity of luminescent organic molecules. Journal of Materials Chemistry C, 2022, 10, 4785-4794.	5.5	12
90	Ultrafast anisotropic x-ray scattering in the condensed phase. New Journal of Physics, 2012, 14, 113002.	2.9	11

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91	Halogen bonding properties of 4-iodopyrazole and 4-bromopyrazole explored by rotational spectroscopy and ab initio calculations. Journal of Chemical Physics, 2017, 147, 214303.	3.0	11
92	A monomeric (trimethylsilyl)methyl lithium complex: synthesis, structure, decomposition and preliminary reactivity studies. Dalton Transactions, 2022, 51, 10707-10713.	3.3	11
93	Solvent rearrangements during the transition from hydrophilic to hydrophobic solvation. Chemical Physics, 2013, 410, 25-30.	1.9	10
94	Circularly polarised luminescence in an RNA-based homochiral, self-repairing, coordination polymer hydrogel. Journal of Materials Chemistry C, 2022, 10, 7329-7335.	5.5	10
95	Probing the dynamics of plasmon-excited hexanethiol-capped gold nanoparticles by picosecond X-ray absorption spectroscopy. Physical Chemistry Chemical Physics, 2014, 16, 23157-23163.	2.8	9
96	Local Control Theory in Trajectory Surface Hopping Dynamics Applied to the Excitedâ€State Proton Transfer of 4â€Hydroxyacridine. ChemPhysChem, 2015, 16, 2127-2133.	2.1	9
97	Accelerating direct quantum dynamics using graphical processing units. Physical Chemistry Chemical Physics, 2017, 19, 19601-19608.	2.8	9
98	On the analysis of X-ray absorption spectra for polyoxometallates. Chemical Physics Letters, 2021, 780, 138893.	2.6	9
99	Enhancing the analysis of disorder in X-ray absorption spectra: application of deep neural networks to T-jump-X-ray probe experiments. Physical Chemistry Chemical Physics, 2021, 23, 9259-9269.	2.8	9
100	The photodissociation of ozone: A quasi-classical approach to a quantum dynamics problem. Journal of Molecular Graphics and Modelling, 2007, 26, 613-621.	2.4	8
101	Ultrafast X-ray Absorption Studies of the Structural Dynamics of Molecular and Biological Systems in Solution. Chimia, 2011, 65, 303-307.	0.6	7
102	Vibrational Coherence Spectroscopy Identifies Ultrafast Branching in an Iron(II) Sensitizer. Journal of Physical Chemistry Letters, 2021, 12, 8560-8565.	4.6	7
103	Hydrophobicity with atomic resolution: Steady-state and ultrafast X-ray absorption and molecular dynamics studies. Pure and Applied Chemistry, 2012, 85, 53-60.	1.9	6
104	Nonadiabatic ab initio molecular dynamics using linear-response time-dependent density functional theory. Open Physics, 2013, 11, .	1.7	6
105	Local Control Theory using Trajectory Surface Hopping and Linear-Response Time-Dependent Density Functional Theory. Chimia, 2013, 67, 218-221.	0.6	6
106	Modeling Molecular Emitters in Organic Light-Emitting Diodes with the Quantum Mechanical Bespoke Force Field. Journal of Chemical Theory and Computation, 2021, 17, 5021-5033.	5.3	6
107	Mechanical (QM/MM) Simulations of Adiabatic and Nonadiabatic Ultrafast Phenomena. Chimia, 2011, 65, 330-333.	0.6	5
108	Real-Time Electron Nanoscopy of Photovoltaic Absorber Formation from Kesterite Nanoparticles. ACS Applied Energy Materials, 2020, 3, 122-128.	5.1	5

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109	Efficient Adversarial Generation of Thermally Activated Delayed Fluorescence Molecules. ACS Omega, 2022, 7, 18179-18188.	3.5	5
110	Using the Mechanical Bond to Tune the Performance of a Thermally Activated Delayed Fluorescence Emitter**. Angewandte Chemie, 2021, 133, 12173-12180.	2.0	4
111	Beyond structural insight: a deep neural network for the prediction of Pt L_{2/3}-edge X-ray absorption spectra. Physical Chemistry Chemical Physics, 2022, 24, 9156-9167.	2.8	4
112	Electronic and non-adiabatic dynamics: general discussion. Faraday Discussions, 2016, 194, 209-257.	3.2	3
113	Intrinsic photogeneration of long-lived charges in a donor-orthogonal acceptor conjugated polymer. Chemical Science, 2021, 12, 8165-8177.	7.4	3
114	Vibrational and condensed phase dynamics: general discussion. Faraday Discussions, 2016, 194, 747-775.	3.2	1
115	Photophysics of Thermally Activated Delayed Fluorescence in Organic Molecules. Materials and Energy, 2018, , 227-261.	0.1	1
116	On assessing functional errors in density functional theory using atomisation energies and electric field gradients. International Journal of Quantum Chemistry, 0, , e26799.	2.0	1
117	Structural dynamics: general discussion. Faraday Discussions, 2016, 194, 583-620.	3.2	0
118	Frontispiece: Luminescent Gold(III) Thiolates: Supramolecular Interactions Trigger and Control Switchable Photoemissions from Bimolecular Excited States. Chemistry - A European Journal, 2017, 23, .	3.3	0
119	Femtosecond X-ray Absorption and Emission Spectroscopy on ZnO Nanoparticles in Solution. , 2016, , .		0
120	Femtosecond Molecular Flattening in [Cu(dmp)2]+ Probed by X-ray Emission Spectroscopy and Solution Scattering. , 2020, , .		0
121	Recent progress and application of computational chemistry to understand inorganic photochemistry. , 2021, , .		0
122	Correction to Inverting the Handedness of Circularly Polarized Luminescence from Light-Emitting Polymers Using Film Thickness. ACS Nano, 2022, 16, 9962-9963.	14.6	0