Thomas J Penfold

List of Publications by Year in Descending Order

116 papers	4,906 citations	36 h-index	68 g-index
130 ext. papers	5,943 ext. citations	6 avg, IF	6.41 L-index

#	Paper	IF	Citations
116	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	3.9	0
115	Circularly polarised luminescence in an RNA-based homochiral, self-repairing, coordination polymer hydrogel. *Journal of Materials Chemistry C*, **2022**, 10, 7329-7335	7.1	1
114	Efficient Adversarial Generation of Thermally Activated Delayed Fluorescence Molecules. *ACS Omega*, **2022**, 7, 18179-18188	3.9	2
113	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	2.8	12
112	Using the Mechanical Bond to Tune the Performance of a Thermally Activated Delayed Fluorescence Emitter*. *Angewandte Chemie - International Edition*, **2021**, 60, 12066-12073	16.4	13
111	Using the Mechanical Bond to Tune the Performance of a Thermally Activated Delayed Fluorescence Emitter**. *Angewandte Chemie*, **2021**, 133, 12173-12180	3.6	2
110	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	6.4	1
109	A quantum dynamics study of the hyperfluorescence mechanism. *Journal of Materials Chemistry C*, **2021**, 9, 1362-1369	7.1	10
108	Influence of Heavy Atom Effect on the Photophysics of Coinage Metal Carbene-Metal-Amide Emitters. *Advanced Functional Materials*, **2021**, 31, 2005438	15.6	11
107	Exceptionally fast radiative decay of a dinuclear platinum complex through thermally activated delayed fluorescence. *Chemical Science*, **2021**, 12, 6172-6180	9.4	14
106	On the factors influencing the chiroptical response of conjugated polymer thin films. *Chemical Communications*, **2021**, 57, 9914-9917	5.8	5
105	Intrinsic photogeneration of long-lived charges in a donor-orthogonal acceptor conjugated polymer. *Chemical Science*, **2021**, 12, 8165-8177	9.4	1
104	A monomeric methyllithium complex: synthesis and structure. *Chemical Communications*, **2021**, 57, 6205-6208	5.8	4
103	Vibrational Coherence Spectroscopy Identifies Ultrafast Branching in an Iron(II) Sensitizer. *Journal of Physical Chemistry Letters*, **2021**, 12, 8560-8565	6.4	2
102	On the analysis of X-ray absorption spectra for polyoxometallates. *Chemical Physics Letters*, **2021**, 780, 138893	2.5	2
101	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	3.6	4
100	Pathways to increase the dissymmetry in the interaction of chiral light and chiral molecules. *Chemical Science*, **2021**, 12, 8589-8602	9.4	39

99	A Deep Neural Network for the Rapid Prediction of X-ray Absorption Spectra. *Journal of Physical Chemistry A*, **2020**, 124, 4263-4270	2.8	30
98	Redox Potentials of Polyoxometalates from an Implicit Solvent Model and QM/MM Molecular Dynamics. *Journal of Physical Chemistry C*, **2020**, 124, 15045-15056	3.8	8
97	The Role of Structural Representation in the Performance of a Deep Neural Network for X-Ray Spectroscopy. *Molecules*, **2020**, 25,	4.8	7
96	Competition between the heavy atom effect and vibronic coupling in donor-bridge-acceptor organometallics. *Physical Chemistry Chemical Physics*, **2020**, 22, 4659-4667	3.6	20
95	Hydrostatic Pressure-Induced Spectral Variation of Reichardt's Dye: A Polarity/Pressure Dual Indicator. *ACS Omega*, **2020**, 5, 897-903	3.9	10
94	Understanding and Designing Thermally Activated Delayed Fluorescence Emitters: Beyond the Energy Gap Approximation. *Chemical Record*, **2020**, 20, 831-856	6.6	24
93	Real-Time Electron Nanoscopy of Photovoltaic Absorber Formation from Kesterite Nanoparticles. *ACS Applied Energy Materials*, **2020**, 3, 122-128	6.1	1
92	Femtosecond X-ray emission study of the spin cross-over dynamics in haem proteins. *Nature Communications*, **2020**, 11, 4145	17.4	12
91	Ultrafast nonadiabatic dynamics probed by nitrogen K-edge absorption spectroscopy. *Physical Chemistry Chemical Physics*, **2020**, 22, 2667-2676	3.6	22
90	Tracking multiple components of a nuclear wavepacket in photoexcited Cu(I)-phenanthroline complex using ultrafast X-ray spectroscopy. *Nature Communications*, **2019**, 10, 3606	17.4	37
89	Simulation of ultrafast excited-state dynamics and elastic x-ray scattering by quantum wavepacket dynamics. *Journal of Chemical Physics*, **2019**, 151, 104307	3.9	13
88	Understanding the potential for efficient triplet harvesting with hot excitons. *Faraday Discussions*, **2019**, 216, 395-413	3.6	10
87	Inverting the Handedness of Circularly Polarized Luminescence from Light-Emitting Polymers Using Film Thickness. *ACS Nano*, **2019**, 13, 8099-8105	16.7	73
86	On the geometry dependence of tuned-range separated hybrid functionals. *Journal of Computational Chemistry*, **2019**, 40, 2191-2199	3.5	12
85	The influence of molecular geometry on the efficiency of thermally activated delayed fluorescence. *Journal of Materials Chemistry C*, **2019**, 7, 6672-6684	7.1	33
84	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	11
83	Excited State Intramolecular Proton Transfer Dynamics for Triplet Harvesting in Organic Molecules. *Journal of Physical Chemistry A*, **2019**, 123, 2640-2649	2.8	13
82	Hydrostatic Pressure-Controlled Ratiometric Luminescence Responses of a Dibenzo[a,j]phenazine-Cored Mechanoluminophore. *ChemPhotoChem*, **2019**, 3, 1203-1211	3.3	21

81	D–A–D TADF emitters: the role of the density of states for achieving faster triplet harvesting rates. *Journal of Materials Chemistry C*, **2019**, 7, 12942-12952	7.1	11
80	Triazatruxene: A Rigid Central Donor Unit for a D-A Thermally Activated Delayed Fluorescence Material Exhibiting Sub-Microsecond Reverse Intersystem Crossing and Unity Quantum Yield via Multiple Singlet-Triplet State Pairs. *Advanced Science*, **2018**, 5, 1700989	13.6	103
79	Revealing hole trapping in zinc oxide nanoparticles by time-resolved X-ray spectroscopy. *Nature Communications*, **2018**, 9, 478	17.4	53
78	Photophysics of Thermally Activated Delayed Fluorescence in Organic Molecules. *Materials and Energy*, **2018**, 227-261		1
77	The intersystem crossing mechanism of an ultrapure blue organoboron emitter. *Organic Electronics*, **2018**, 59, 45-48	3.5	28
76	Spin-Vibronic Mechanism for Intersystem Crossing. *Chemical Reviews*, **2018**, 118, 6975-7025	68.1	377
75	The theory of thermally activated delayed fluorescence for organic light emitting diodes. *Chemical Communications*, **2018**, 54, 3926-3935	5.8	159
74	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	5.1	23
73	The influence of molecular conformation on the photophysics of organic room temperature phosphorescent luminophores. *Journal of Materials Chemistry C*, **2018**, 6, 9238-9247	7.1	42
72	Non-equilibrium x-ray spectroscopy using direct quantum dynamics. *Journal of Chemical Physics*, **2018**, 149, 124107	3.9	14
71	The Role of Vibronic Coupling for Intersystem Crossing and Reverse Intersystem Crossing Rates in TADF Molecules **2018**, 297-330		2
70	The intersystem crossing of a cyclic (alkyl)(amino) carbene gold (i) complex. *Journal of Chemical Physics*, **2018**, 149, 014304	3.9	40
69	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	6.4	10
68	Investigating interfacial electron transfer in dye-sensitized NiO using vibrational spectroscopy. *Physical Chemistry Chemical Physics*, **2017**, 19, 7877-7885	3.6	18
67	Photophysics of thermally activated delayed fluorescence molecules. *Methods and Applications in Fluorescence*, **2017**, 5, 012001	3.1	265
66	Nonadiabatic coupling reduces the activation energy in thermally activated delayed fluorescence. *Physical Chemistry Chemical Physics*, **2017**, 19, 8428-8434	3.6	94
65	Regio- and conformational isomerization critical to design of efficient thermally-activated delayed fluorescence emitters. *Nature Communications*, **2017**, 8, 14987	17.4	179
64	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	16.4	32

63	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	7.1	65
62	Accelerating direct quantum dynamics using graphical processing units. *Physical Chemistry Chemical Physics*, **2017**, 19, 19601-19608	3.6	7
61	Photophysics of a copper phenanthroline elucidated by trajectory and wavepacket-based quantum dynamics: a synergetic approach. *Physical Chemistry Chemical Physics*, **2017**, 19, 19590-19600	3.6	32
60	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	7.1	84
59	Circularly Polarised Luminescence from Helically Chiral Confused N,N,O,C-Boron-Chelated Dipyrromethenes (BODIPYs). *ChemPhotoChem*, **2017**, 1, 513-517	3.3	41
58	Structural Diversity and Argentophilic Interactions in One-Dimensional Silver-Based Coordination Polymers. *Crystal Growth and Design*, **2017**, 17, 5753-5763	3.5	13
57	Luminescent Gold(III) Thiolates: Supramolecular Interactions Trigger and Control Switchable Photoemissions from Bimolecular Excited States. *Chemistry - A European Journal*, **2017**, 23, 105-113	4.8	37
56	Halogen bonding properties of 4-iodopyrazole and 4-bromopyrazole explored by rotational spectroscopy and ab initio calculations. *Journal of Chemical Physics*, **2017**, 147, 214303	3.9	7
55	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	3.8	26
54	The Importance of Vibronic Coupling for Efficient Reverse Intersystem Crossing in Thermally Activated Delayed Fluorescence Molecules. *ChemPhysChem*, **2016**, 17, 2956-2961	3.2	404
53	Establishing nonlinearity thresholds with ultraintense X-ray pulses. *Scientific Reports*, **2016**, 6, 33292	4.9	36
52	Structural dynamics: general discussion. *Faraday Discussions*, **2016**, 194, 583-620	3.6	
51	Vibrational and condensed phase dynamics: general discussion. *Faraday Discussions*, **2016**, 194, 747-775	3.6	1
50	Electronic and non-adiabatic dynamics: general discussion. *Faraday Discussions*, **2016**, 194, 209-257	3.6	3
49	Revealing the spin-vibronic coupling mechanism of thermally activated delayed fluorescence. *Nature Communications*, **2016**, 7, 13680	17.4	468
48	High-Efficiency Iron Photosensitizer Explained with Quantum Wavepacket Dynamics. *Journal of Physical Chemistry Letters*, **2016**, 7, 2009-14	6.4	49
47	Probing spin-vibronic dynamics using femtosecond X-ray spectroscopy. *Faraday Discussions*, **2016**, 194, 731-746	3.6	15
46	Investigating DNA Radiation Damage Using X-Ray Absorption Spectroscopy. *Biophysical Journal*, **2016**, 110, 1304-11	2.9	11

45	Theoretical Rationalization of the Emission Properties of Prototypical Cu(I)-Phenanthroline Complexes. *Journal of Physical Chemistry A*, **2015**, 119, 7026-37	2.8	43
44	Synthesis and luminescence modulation of pyrazine-based gold(III) pincer complexes. *Chemical Communications*, **2015**, 51, 16629-32	5.8	67
43	Local Control Theory in Trajectory Surface Hopping Dynamics Applied to the Excited-State Proton Transfer of 4-Hydroxyacridine. *ChemPhysChem*, **2015**, 16, 2127-33	3.2	8
42	Identifying the major intermediate species by combining time-resolved X-ray solution scattering and X-ray absorption spectroscopy. *Physical Chemistry Chemical Physics*, **2015**, 17, 23298-302	3.6	13
41	Ultrafast core-loss spectroscopy in four-dimensional electron microscopy. *Structural Dynamics*, **2015**, 2, 024302	3.2	45
40	Probing wavepacket dynamics using ultrafast x-ray spectroscopy. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2015**, 48, 214001	1.3	37
39	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, 12922-7	11.5	28
38	On Predicting the Excited-State Properties of Thermally Activated Delayed Fluorescence Emitters. *Journal of Physical Chemistry C*, **2015**, 119, 13535-13544	3.8	125
37	Recent experimental and theoretical developments in time-resolved X-ray spectroscopies. *Coordination Chemistry Reviews*, **2014**, 277-278, 44-68	23.2	142
36	Derivation of spin-orbit couplings in collinear linear-response TDDFT: a rigorous formulation. *Journal of Chemical Physics*, **2014**, 140, 144103	3.9	39
35	Mapping of the photoinduced electron traps in TiO by picosecond X-ray absorption spectroscopy. *Angewandte Chemie - International Edition*, **2014**, 53, 5858-62	16.4	83
34	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, 1617-31	3.6	32
33	Probing the dynamics of plasmon-excited hexanethiol-capped gold nanoparticles by picosecond X-ray absorption spectroscopy. *Physical Chemistry Chemical Physics*, **2014**, 16, 23157-63	3.6	8
32	X-ray spectroscopic study of solvent effects on the ferrous and ferric hexacyanide anions. *Journal of Physical Chemistry A*, **2014**, 118, 9411-8	2.8	33
31	A quantum dynamics study of the ultrafast relaxation in a prototypical Cu(I)-phenanthroline. *Journal of Physical Chemistry A*, **2014**, 118, 9861-9	2.8	62
30	Characterizing the Structure and Defect Concentration of ZnO Nanoparticles in a Colloidal Solution. *Journal of Physical Chemistry C*, **2014**, 118, 19422-19430	3.8	14
29	Photooxidation and photoaquation of iron hexacyanide in aqueous solution: A picosecond X-ray absorption study. *Structural Dynamics*, **2014**, 1, 024901	3.2	41
28	Mapping of the Photoinduced Electron Traps in TiO2 by Picosecond X-ray Absorption Spectroscopy. *Angewandte Chemie*, **2014**, 126, 5968-5972	3.6	13

27	A vibronic coupling hamiltonian to describe the ultrafast excited state dynamics of a Cu(i)-phenanthroline complex. *Chimia*, **2014**, 68, 227-30	1.3	30
26	The role of Hartree□Fock exchange in the simulation of X-ray absorption spectra: A study of photoexcited. *Chemical Physics Letters*, **2013**, 580, 179-184	2.5	36
25	Nonadiabatic ab initio molecular dynamics using linear-response time-dependent density functional theory. *Open Physics*, **2013**, 11,	1.3	4
24	X-ray absorption spectroscopy of ground and excited rhenium-carbonyl-diimine complexes: evidence for a two-center electron transfer. *Journal of Physical Chemistry A*, **2013**, 117, 361-9	2.8	57
23	A wavelet analysis for the X-ray absorption spectra of molecules. *Journal of Chemical Physics*, **2013**, 138, 014104	3.9	32
22	Solvent rearrangements during the transition from hydrophilic to hydrophobic solvation. *Chemical Physics*, **2013**, 410, 25-30	2.3	8
21	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, 4591-601	2.8	95
20	Local control theory using trajectory surface hopping and linear-response time-dependent density functional theory. *Chimia*, **2013**, 67, 218-21	1.3	6
19	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, 5603-8	11.5	28
18	Simulations of X-ray absorption spectra: the effect of the solvent. *Physical Chemistry Chemical Physics*, **2012**, 14, 9444-50	3.6	20
17	A femtosecond fluorescence study of vibrational relaxation and cooling dynamics of UV dyes. *Physical Chemistry Chemical Physics*, **2012**, 14, 3513-9	3.6	59
16	Ultrafast anisotropic x-ray scattering in the condensed phase. *New Journal of Physics*, **2012**, 14, 113002	2.9	10
15	Hydrophobicity with atomic resolution: Steady-state and ultrafast X-ray absorption and molecular dynamics studies. *Pure and Applied Chemistry*, **2012**, 85, 53-60	2.1	5
14	Quantum dynamics study of the competing ultrafast intersystem crossing and internal conversion in the "channel 3" region of benzene. *Journal of Chemical Physics*, **2012**, 137, 204310	3.9	30
13	Probing the transition from hydrophilic to hydrophobic solvation with atomic scale resolution. *Journal of the American Chemical Society*, **2011**, 133, 12740-8	16.4	66
12	Mixed quantum mechanical/molecular mechanical (QM/MM) simulations of adiabatic and nonadiabatic ultrafast phenomena. *Chimia*, **2011**, 65, 330-3	1.3	5
11	Ultrafast X-ray absorption studies of the structural dynamics of molecular and biological systems in solution. *Chimia*, **2011**, 65, 303-7	1.3	7
10	Pushing the frontiers of first-principles based computer simulations of chemical and biological systems. *Chimia*, **2011**, 65, 667-71	1.3	16

9	Local control theory in trajectory-based nonadiabatic dynamics. *Physical Review A*, **2011**, 84,	2.6	22
8	Local control of multidimensional dynamics. *Physical Chemistry Chemical Physics*, **2010**, 12, 15616-27	3.6	26
7	Competing ultrafast intersystem crossing and internal conversion in the "channel 3" region of benzene. *Physical Chemistry Chemical Physics*, **2010**, 12, 15607-15	3.6	91
6	The effect of molecular distortions on spin□rbit coupling in simple hydrocarbons. *Chemical Physics*, **2010**, 375, 58-66	2.3	42
5	Ultrafast dynamics of the S1 excited state of benzene. *Chemical Physics Letters*, **2009**, 469, 43-47	2.5	76
4	A model Hamiltonian to simulate the complex photochemistry of benzene II. *Journal of Chemical Physics*, **2009**, 131, 064303	3.9	32
3	The photodissociation of ozone: a quasi-classical approach to a quantum dynamics problem. *Journal of Molecular Graphics and Modelling*, **2007**, 26, 613-21	2.8	8
2	On assessing functional errors in density functional theory using atomisation energies and electric field gradients. *International Journal of Quantum Chemistry*,e26799	2.1	
1	Recent Advances in Ultrafast X-Ray Absorption Spectroscopy of Solutions. *Advances in Chemical Physics*,1-41		14