

Jeremy G. Frey

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

145 papers	2,180 citations	24 h-index	40 g-index
176 ext. papers	2,454 ext. citations	5 avg, IF	4.68 L-index

#	Paper	IF	Citations
145	Artificial Intelligence and Chemistry. <i>Chemistry International</i> , 2022 , 44, 6-9	1.6	0
144	Artificial intelligence and ethics within the food sector: Developing a common language for technology adoption across the supply chain. <i>Trends in Food Science and Technology</i> , 2022 , 125, 33-42	15.3	0
143	Considering the ethical implications of digital collaboration in the Food Sector. <i>Patterns</i> , 2021 , 2, 100335	5.1	1
142	Canine mammary cancer tumour behaviour and patient survival time are associated with collagen fibre characteristics. <i>Scientific Reports</i> , 2021 , 11, 5668	4.9	0
141	Semantic Technologies in Drug Discovery 2021 , 129-144		1
140	The AI for Scientific Discovery Network. <i>Patterns</i> , 2021 , 2, 100162	5.1	1
139	A trust framework for digital food systems. <i>Nature Food</i> , 2021 , 2, 543-545	14.4	2
138	Quantitative and correlative extreme ultraviolet coherent imaging of mouse hippocampal neurons at high resolution. <i>Science Advances</i> , 2020 , 6, eaaz3025	14.3	11
137	. <i>IEEE Internet of Things Journal</i> , 2020 , 7, 8631-8640	10.7	4
136	Taking FAIR on the ChIN: The Chemistry Implementation Network. <i>Data Intelligence</i> , 2020 , 2, 131-138	3	7
135	Canine mammary cancer diagnosis from quantitative properties of nonlinear optical images. <i>Biomedical Optics Express</i> , 2020 , 11, 6413-6427	3.5	2
134	. <i>IEEE Sensors Journal</i> , 2019 , 19, 2984-2990	4	1
133	A new wave of innovation in Semantic web tools for drug discovery. <i>Expert Opinion on Drug Discovery</i> , 2019 , 14, 433-444	6.2	13
132	Are Distributed Ledger Technologies the panacea for food traceability?. <i>Global Food Security</i> , 2019 , 20, 145-149	8.3	82
131	Too many tags spoil the metadata: investigating the knowledge management of scientific research with semantic web technologies. <i>Journal of Cheminformatics</i> , 2019 , 11, 23	8.6	5
130	A new topological descriptor for water network structure. <i>Journal of Cheminformatics</i> , 2019 , 11, 48	8.6	6
129	Unexpected finite size effects in interfacial systems: Why bigger is not always better-Increase in uncertainty of surface tension with bulk phase width. <i>Journal of Chemical Physics</i> , 2018 , 148, 214704	3.9	5

128	Improved understanding of aqueous solubility modeling through topological data analysis. <i>Journal of Cheminformatics</i> , 2018 , 10, 54	8.6	8
127	Surface reconstruction amendment to the intrinsic sampling method. <i>Journal of Chemical Physics</i> , 2018 , 149, 234705	3.9	2
126	Efficient high-harmonic generation from a stable and compact ultrafast Yb-fiber laser producing 100fs, 350fs pulses based on bendable photonic crystal fiber. <i>Applied Physics B: Lasers and Optics</i> , 2017 , 123, 43	1.9	13
125	Electronic lab notebooks: can they replace paper?. <i>Journal of Cheminformatics</i> , 2017 , 9, 31	8.6	29
124	Quantitative Evaluation of Hard X-ray Damage to Biological Samples using EUV Ptychography. <i>Journal of Physics: Conference Series</i> , 2017 , 849, 012034	0.3	1
123	Connecting Chemistry with Global Challenges through Data Standards. <i>Chemistry International</i> , 2017 , 39, 5-8	1.6	2
122	Ptychographic coherent diffractive imaging with orthogonal probe relaxation. <i>Optics Express</i> , 2016 , 24, 8360-9	3.3	43
121	Effects of using structured templates for recalling chemistry experiments. <i>Journal of Cheminformatics</i> , 2016 , 8, 9	8.6	2
120	QSAR analysis of substituent effects on tambjamine anion transporters. <i>Chemical Science</i> , 2016 , 7, 1600-1608	9.4	36
119	Wide-field broadband extreme ultraviolet transmission ptychography using a high-harmonic source: publisher's note. <i>Optics Letters</i> , 2016 , 41, 3057	3	
118	Lloyd's mirror interference lithography with EUV radiation from a high-harmonic source. <i>Applied Physics Express</i> , 2016 , 9, 076701	2.4	3
117	Wide-field broadband extreme ultraviolet transmission ptychography using a high-harmonic source. <i>Optics Letters</i> , 2016 , 41, 1317-20	3	19
116	Experiences with a researcher-centric ELN. <i>Chemical Science</i> , 2015 , 6, 1614-1629	9.4	18
115	The Evolution of Digital Chemistry at Southampton. <i>Molecular Informatics</i> , 2015 , 34, 585-97	3.8	2
114	Data Science Professional Uncovered: How the EDISON Project will Contribute to a Widely Accepted Profile for Data Scientists 2015 ,		27
113	Ultra-broadband ptychography with self-consistent coherence estimation from a high harmonic source 2015 ,		2
112	ChemTrove: enabling a generic ELN to support chemistry through the use of transferable plug-ins and online data sources. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 501-9	6.1	8
111	User-Defined Metadata: Using Cues and Changing Perspectives. <i>International Journal of Digital Curation</i> , 2015 , 10, 18-47	0.9	3

110	Collection, Curation, Citation at Source: Publication@Source 10 Years On. <i>International Journal of Digital Curation</i> , 2015 , 10, 1-11	0.9	4
109	Monolayer detection of ion binding at a crown ether-functionalised supramolecular surface via an integrated optical Bragg grating. <i>Analyst, The</i> , 2014 , 139, 2774-82	5	4
108	High-energy laser-pulse self-compression in short gas-filled fibers. <i>Physical Review A</i> , 2014 , 89,	2.6	9
107	Usage and applications of Semantic Web techniques and technologies to support chemistry research. <i>Journal of Cheminformatics</i> , 2014 , 6, 18	8.6	2
106	Digital IUPAC. <i>Chemistry International</i> , 2014 , 36,	1.6	4
105	Creating context for the experiment record. User-defined metadata: investigations into metadata usage in the LabTrove ELN. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 3268-83	6.1	8
104	Scientific and technical data sharing: a trading perspective. <i>Journal of Computer-Aided Molecular Design</i> , 2014 , 28, 989-96	4.2	3
103	Laboratory notebooks in the digital era: the role of ELNs in record keeping for chemistry and other sciences. <i>Chemical Society Reviews</i> , 2013 , 42, 8157-75	58.5	32
102	First steps towards semantic descriptions of electronic laboratory notebook records. <i>Journal of Cheminformatics</i> , 2013 , 5, 52	8.6	21
101	Ultra-broadband support determination for extreme ultraviolet coherent diffractive imaging from a high harmonic source. <i>Journal of Optics (United Kingdom)</i> , 2013 , 15, 094009	1.7	8
100	Cheminformatics and the Semantic Web: adding value with linked data and enhanced provenance. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2013 , 3, 465-481	7.9	19
99	Bright extreme-ultraviolet high-order-harmonic radiation from optimized pulse compression in short hollow waveguides. <i>Physical Review A</i> , 2013 , 87,	2.6	8
98	Towards predictable transmembrane transport: QSAR analysis of anion binding and transport. <i>Chemical Science</i> , 2013 , 4, 3036	9.4	89
97	Chemical information matters: an e-Research perspective on information and data sharing in the chemical sciences. <i>Chemical Society Reviews</i> , 2013 , 42, 6754-76	58.5	31
96	Enhancing research publications using Rich Interactive Narratives. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2013 , 371, 20120090	3	2
95	MyExperimentalScience, extending the workflow. <i>Concurrency Computation Practice and Experience</i> , 2013 , 25, 481-496	1.4	5
94	Temporal Coherence Effects on Coherent Diffractive Imaging of a Binary Sample by a High Harmonic Source. <i>EPJ Web of Conferences</i> , 2013 , 41, 12015	0.3	
93	LabTrove: a lightweight, web based, laboratory "blog" as a route towards a marked up record of work in a bioscience research laboratory. <i>PLoS ONE</i> , 2013 , 8, e67460	3.7	20

92	Data Curation Issues in the Chemical Sciences. <i>Information Standards Quarterly</i> , 2013 , 25, 4		4
91	Spatiotemporal phase-matching in capillary high-harmonic generation. <i>Journal of the Optical Society of America B: Optical Physics</i> , 2012 , 29, 806	1.7	3
90	Web-based services for drug design and discovery. <i>Expert Opinion on Drug Discovery</i> , 2011 , 6, 885-95	6.2	9
89	Gas jet structure influence on high harmonic generation. <i>Optics Express</i> , 2011 , 19, 9801-6	3.3	2
88	Crown ethers at the aqueous solution-air interface: 1. Assignments and surface spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 7930-8	3.6	3
87	Crown ethers at the aqueous solution-air interface. Part 2. Electrolyte effects, ethylene oxide hydration and temperature behaviour. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 7939-47	3.6	
86	Modal effects on pump-pulse propagation in an Ar-filled capillary. <i>Optics Express</i> , 2010 , 18, 13279-84	3.3	10
85	A Semantic eScience Platform for Chemistry 2010 ,		8
84	The smartLab: Experimental and environmental control and monitoring of the chemistry laboratory 2009 ,		2
83	Spatially resolved Ar* and Ar ⁺ imaging as a diagnostic for capillary-based high harmonic generation. <i>Journal of Optics</i> , 2009 , 11, 054011		1
82	The value of the Semantic Web in the laboratory. <i>Drug Discovery Today</i> , 2009 , 14, 552-61	8.8	19
81	EUV off-axis focusing using a high harmonic source 2009 ,		2
80	Combining System Introspection with User-Provided Description to Support Configuration and Understanding of Pervasive systems 2008 ,		2
79	Molecular variation of capillary-produced soft x-ray high harmonics. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2008 , 41, 145602	1.3	2
78	Direct measurement of the complex refractive index in the extreme ultraviolet spectral region using diffraction from a nanosphere array. <i>Applied Physics Letters</i> , 2008 , 93, 231103	3.4	9
77	The water-like film on water. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2008 , 5, 1184-1186		9
76	Adsorption of rhodamine 6G at the water-air interface. <i>Physica Status Solidi C: Current Topics in Solid State Physics</i> , 2008 , 5, 1187-1189		2
75	e-Malaria: the schools Malaria project. <i>Concurrency Computation Practice and Experience</i> , 2008 , 20, 225-238		1

74	Curation of Laboratory Experimental Data as Part of the Overall Data Lifecycle. <i>International Journal of Digital Curation</i> , 2008 , 3, 44-62	0.9	13
73	Spatially resolved soft X-ray spectrometry from single-image diffraction. <i>Nature Physics</i> , 2007 , 3, 176-179	6.2	7
72	High-Throughput Structure/Function Screening of Materials and Catalysts with Multiple Spectroscopic Techniques. <i>AIP Conference Proceedings</i> , 2007 ,	0	3
71	Reflection second harmonic generation on a z-cut congruent lithium niobate crystal. <i>Physical Review B</i> , 2006 , 74,	3.3	13
70	A computer-aided drug discovery system for chemistry teaching. <i>Journal of Chemical Information and Modeling</i> , 2006 , 46, 960-70	6.1	8
69	An e-science environment for service crystallography--from submission to dissemination. <i>Journal of Chemical Information and Modeling</i> , 2006 , 46, 1006-16	6.1	33
68	Soft-x-ray wavelength shift induced by ionization effects in a capillary. <i>Optics Letters</i> , 2006 , 31, 374-6	3	46
67	Multiphoton transitions for the harmonic oscillator. <i>Molecular Physics</i> , 2006 , 104, 2523-2525	1.7	
66	Mass transfer enhancement produced by laser induced cavitation. <i>Electrochemistry Communications</i> , 2006 , 8, 1603-1609	5.1	11
65	The Semantic Grid and chemistry: Experiences with CombeChem. <i>Web Semantics</i> , 2006 , 4, 84-101	2.9	19
64	Bringing chemical data onto the Semantic Web. <i>Journal of Chemical Information and Modeling</i> , 2006 , 46, 939-52	6.1	42
63	A semantic datagrid for combinatorial chemistry 2005 ,		6
62	Resin bead micro-UV-visible absorption spectroscopy. <i>Analytical Chemistry</i> , 2005 , 77, 2247-51	7.8	10
61	Prediction of properties from simulations: a re-examination with modern statistical methods. <i>Journal of Chemical Information and Modeling</i> , 2005 , 45, 1791-803	6.1	8
60	Generalized ultrafast dispersion scans of continuum generation induced by sub-50fs chirped pulses in highly nonlinear tapered planar waveguides 2005 , 5714, 200		1
59	Grid computing and biomolecular simulation. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2005 , 363, 2017-35	3	16
58	Grid-based dynamic electronic publication: a case study using combined experiment and simulation studies of crown ethers at the air/water interface. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2005 , 363, 2075-95	3	5
57	Statistical analysis of second harmonic generation experiments: a phenomenological model. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2005 , 75, 45-54	3.8	2

56	ECSES [Examining crystal structures using 'e-science': a demonstrator employing web and grid services to enhance user participation in crystallographic experiments. <i>Journal of Applied Crystallography</i> , 2005 , 38, 819-826	3.8	9
55	Second Harmonic Generation at Liquid/Liquid Interfaces 2005 , 1-23		
54	Making tea 2004 ,		12
53	The semantic smart laboratory: a system for supporting the chemical eScientist. <i>Organic and Biomolecular Chemistry</i> , 2004 , 2, 3284-93	3.9	35
52	Probing possible structural models at the air/H ₂ SO ₄ (aq) interface: a second harmonic generation study. <i>Physical Chemistry Chemical Physics</i> , 2004 , 6, 2415	3.6	2
51	Dark Lab or Smart Lab: The Challenges for 21st Century Laboratory Software. <i>Organic Process Research and Development</i> , 2004 , 8, 1024-1035	3.9	17
50	Which sites react first? Functional site distribution and kinetics on solid supports investigated using confocal Raman and fluorescence microscopy. <i>ACS Combinatorial Science</i> , 2003 , 5, 28-32		23
49	Anion-directed assembly: the first fluoride-directed double helix. <i>Chemical Communications</i> , 2003 , 568-95.8		141
48	Second harmonic ellipsometry. <i>Measurement Science and Technology</i> , 2003 , 14, 508-515	2	9
47	Enzyme accessibility and solid supports: which molecular weight enzymes can be used on solid supports? An investigation using confocal Raman microscopy. <i>Chemistry - A European Journal</i> , 2002 , 8, 3769-72	4.8	68
46	Synthesis of guanidinium-derived receptor libraries and screening for selective peptide receptors in water. <i>Chemistry - A European Journal</i> , 2002 , 8, 1300-9	4.8	58
45	Synthesis, Conformational Studies and Binding Properties of Acyclic Receptors for N-Protected Amino Acids and Dipeptides. <i>European Journal of Organic Chemistry</i> , 2001 , 2001, 4625	3.2	7
44	Site distribution in resin beads as determined by confocal Raman spectroscopy. <i>Chemistry - A European Journal</i> , 2001 , 7, 3880-3	4.8	25
43	Enantioselective binding of dipeptides using acyclic receptors. <i>Chemical Communications</i> , 2001 , 1358-1359	3.9	15
42	The temperature dependence of surface second-harmonic generation from the air-water interface. <i>Molecular Physics</i> , 2001 , 99, 677-687	1.7	34
41	Interfacial second harmonic generation in the limit of weak orientational order: determining interfacial refractive index. <i>Chemical Physics Letters</i> , 2000 , 323, 454-459	2.5	10
40	Surface second harmonic generation studies of the dodecane/water interface: the equilibrium and kinetic behaviour of p-nitrophenol and tri-n-butyl phosphate. <i>Physical Chemistry Chemical Physics</i> , 2000 , 2, 3235-3245	3.6	22
39	Rayleigh Scattering of Laser and Synchrotron Radiation from Pulsed Free Jets of Ar _n and (N ₂ O) _n Clusters. <i>Journal of Physical Chemistry A</i> , 1998 , 102, 6457-6463	2.8	24

38	Tagging in combinatorial chemistry: the use of coloured and fluorescent beads. <i>Chemical Communications</i> , 1997 , 735-736	5.8	56
37	Investigation of transport across an immiscible liquid/liquid interface. Electrochemical and second harmonic generation studies. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1996 , 92, 1369		22
36	Photodissociation of CS ₂ at 193 nm investigated by polarised photofragment translational spectroscopy. <i>Chemical Physics</i> , 1996 , 202, 397-406	2.3	21
35	Second harmonic generation from the air/water interface of an aqueous solution of the dipeptide Boc-Trp-Trp. <i>Chemical Physics Letters</i> , 1994 , 230, 260-264	2.5	48
34	Ultraviolet photolysis of HOCl: REMPI measurement of the relative population of chlorine atom (2P) spin-orbit states. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1994 , 90, 17-21		13
33	Photolysis of HOBr and DOBr at 266 nm: OH and OD product-state distributions. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1994 , 90, 817		2
32	266 nm Photolysis of HOCl and DOCl: laser-excitation fluorescence detection of OH and OD. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1993 , 89, 1623		19
31	Analysis of time-of-flight data constraints and error bars. <i>Molecular Physics</i> , 1993 , 79, 1287-1303	1.7	2
30	The analysis of anisotropic photodissociation time-of-flight data obtained from a rotating source machine. <i>Molecular Physics</i> , 1992 , 75, 1419-1434	1.7	13
29	Second harmonic generation by p-nitrophenol at water/air and water/heptane interfaces. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1992 , 88, 2027		25
28	Ab initio calculations on the ground and low-lying electronic states of the Cl ₃ radical: emission from Cl ₃ . <i>Chemical Physics Letters</i> , 1992 , 189, 297-302	2.5	7
27	The 248 nm photodissociation of DOCl: laser excitation fluorescence spectra of OD. <i>Chemical Physics Letters</i> , 1991 , 185, 101-104	2.5	13
26	The collision of electronically excited Ba (6s6p 1P ₁) with CO ₂ and H ₂ O clusters. <i>Chemical Physics Letters</i> , 1991 , 176, 325-328	2.5	5
25	A further structural examination of PVC gels. <i>Materials Letters</i> , 1991 , 11, 105-108	3.3	0
24	Raman emission from the photolysis of NOCl at 266 nm. <i>Molecular Physics</i> , 1990 , 69, 943-945	1.7	10
23	Calculation of non-adiabatic matrix elements. <i>Molecular Physics</i> , 1990 , 69, 783-785	1.7	
22	Adiabatic and diabatic representations, coordinate and unitary transformations: coupled oscillators. <i>Molecular Physics</i> , 1990 , 71, 659-665	1.7	
21	Interferometric measurements of the dipole polarizability of molecules between 300 K and 1100 K. <i>Molecular Physics</i> , 1990 , 69, 803-817	1.7	98

20	Three-particle hyperspherical coordinates: permutation-inversion symmetry properties. <i>Molecular Physics</i> , 1990 , 70, 145-159	1.7	9
19	Photolysis of HOCl at 248 nm in a supersonic molecular beam: laser-induced fluorescence spectra of OH. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1990 , 86, 3831		19
18	Energy dependence of the inelastic process Ba(6s6p1P1)+Ar,He-Ba(6s6p3P1,2)+Ar,He. <i>Journal of Chemical Physics</i> , 1990 , 93, 5354-5355	3.9	21
17	Isomerization of cis-stilbene in rare-gas clusters: direct measurements of trans-stilbene formation rates on a picosecond time scale. <i>Journal of the Optical Society of America B: Optical Physics</i> , 1990 , 7, 1540	1.7	25
16	Raman spectra of NOCl and Cl ₂ photodissociation dynamics. <i>Molecular Physics</i> , 1989 , 67, 465-472	1.7	15
15	Adiabatic and diabatic approaches to bound state calculations. <i>Molecular Physics</i> , 1988 , 65, 1313-1320	1.7	4
14	Non-adiabatic corrections for coupled oscillators using Rayleigh-Schrödinger perturbation theory. <i>Molecular Physics</i> , 1988 , 64, 191-206	1.7	8
13	An accurate calculation of the ground state energy of the helium atom and the hydrogen negative ion using hyperspherical coordinates. <i>Chemical Physics</i> , 1987 , 111, 33-36	2.3	18
12	The adiabatic approach to e + 2 e - in the hyperspherical coordinates. <i>Molecular Physics</i> , 1986 , 57, 1-6	1.7	5
11	The calculation of the ground state energy of weakly bound van der waals trimers using the method of hyperspherical harmonics I. The Born-Oppenheimer and adiabatic approximations. <i>Chemical Physics</i> , 1985 , 99, 415-426	2.3	29
10	The calculation of the ground state energy of weakly bound van der waals trimers using the method of hyperspherical harmonics.. <i>Chemical Physics</i> , 1985 , 99, 427-435	2.3	19
9	Infrared predissociation spectra of water dimer in a supersonic molecular beam. <i>Chemical Physics Letters</i> , 1984 , 106, 373-376	2.5	138
8	Excited vibrational states near dissociation in weakly bound triatomic systems. <i>Chemical Physics Letters</i> , 1983 , 102, 421-424	2.5	4
7	Synthesis, structure, and magnetism of a new type of .pi.-molecular complex containing binuclear copper(II) complexes and benzene: bis[2,2-dimethyl-7-(phenylimino)-3,5,7-octanetrionato]dicopper(II)-benzene and bis[2,2-dimethyl-7-[(4-nitrophenyl)imino]-3,5,7-octanetrionato]dicopper(II) bis(benzene). <i>Inorganic Chemistry</i> , 1983 , 22, 121-124	5.1	12
6	Thermal decomposition of 3-ethyl-3-methyloxetan and 3,3-diethyloxetan. <i>Journal of the Chemical Society Faraday Transactions I</i> , 1975 , 71, 2485		3
5			8
4	Grid-enabling an existing instrument-based national service		2
3	The Collaborative Semantic Grid		1

2 Combinatorial Chemistry and the Grid945-962

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1 Data management matters

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