

# Stephen R Elliott

## 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.

86 papers	1,826 citations	26 h-index	40 g-index
90 ext. papers	2,245 ext. citations	7.3 avg, IF	5.34 L-index

#	Paper	IF	Citations
86	Robust Design of High-Performance Optoelectronic Chalcogenide Crystals from High-Throughput Computation.. <i>Journal of the American Chemical Society</i> , <b>2022</b> ,	16.4	4
85	Electric-field-induced annihilation of localized gap defect states in amorphous phase-change memory materials. <i>Acta Materialia</i> , <b>2021</b> , 223, 117465	8.4	1
84	Real-time bioprocess monitoring using a mid-infrared fibre-optic sensor. <i>Biochemical Engineering Journal</i> , <b>2021</b> , 167, 107889	4.2	4
83	On the Chemical Bonding of Amorphous Sb <sub>2</sub> Te <sub>3</sub> . <i>Physica Status Solidi - Rapid Research Letters</i> , <b>2021</b> , 15, 2000485	2.5	6
82	Crystallization of Phase-Change Chalcogenides <b>2021</b> , 367-402		
81	Multi-Center Hyperbonding in Phase-Change Materials. <i>Physica Status Solidi - Rapid Research Letters</i> , <b>2021</b> , 15, 2000516	2.5	3
80	Novel metal oxides with promising high-temperature thermoelectric performance. <i>Journal of Materials Chemistry C</i> , <b>2021</b> , 9, 12884-12894	7.1	1
79	Origins of structural and electronic transitions in disordered silicon. <i>Nature</i> , <b>2021</b> , 589, 59-64	50.4	66
78	Cerebral Microdialysate Metabolite Monitoring using Mid-infrared Spectroscopy. <i>Analytical Chemistry</i> , <b>2021</b> , 93, 11929-11936	7.8	3
77	Antibonding-Induced Anomalous Temperature Dependence of the Band Gap in Crystalline Ge <sub>2</sub> Sb <sub>2</sub> Te <sub>5</sub> . <i>Journal of Physical Chemistry C</i> , <b>2021</b> , 125, 19537-19543	3.8	2
76	ChemDataExtractor 2.0: Autopopulated Ontologies for Materials Science. <i>Journal of Chemical Information and Modeling</i> , <b>2021</b> , 61, 4280-4289	6.1	7
75	A fast, low-energy multi-state phase-change artificial synapse based on uniform partial-state transitions. <i>APL Materials</i> , <b>2021</b> , 9, 091103	5.7	4
74	Quasilocalized Vibrations in Vitreous Silica. <i>Physica Status Solidi (B): Basic Research</i> , <b>2020</b> , 258, 2000422	1.3	
73	Vacancy formation energy and its connection with bonding environment in solid: A high-throughput calculation and machine learning study. <i>Computational Materials Science</i> , <b>2020</b> , 183, 109803	3.2	8
72	Chemical Bonding in Chalcogenides: The Concept of Multicenter Hyperbonding. <i>Advanced Materials</i> , <b>2020</b> , 32, e2000340	24	21
71	Disorder by design: A data-driven approach to amorphous semiconductors without total-energy functionals. <i>Scientific Reports</i> , <b>2020</b> , 10, 7742	4.9	4
70	Elucidation of the Nature of Structural Relaxation in Glassy d-Sorbitol. <i>Journal of Physical Chemistry B</i> , <b>2020</b> , 124, 1833-1838	3.4	0

69	Nonequilibrium ab initio molecular-dynamics simulations of lattice thermal conductivity in irradiated glassy Ge <sub>2</sub> Sb <sub>2</sub> Te <sub>5</sub> . <i>Applied Physics Letters</i> , <b>2020</b> , 116, 031902	3.4	2
68	Synergy effect of co-doping Sc and Y in Sb <sub>2</sub> Te <sub>3</sub> for phase-change memory. <i>Journal of Materials Chemistry C</i> , <b>2020</b> , 8, 6672-6679	7.1	16
67	Temperature-induced nanostructural evolution of hydrogen-rich voids in amorphous silicon: a first-principles study. <i>Nanoscale</i> , <b>2020</b> , 12, 1464-1477	7.7	1
66	Two-dimensional molybdenum carbides: active electrocatalysts for the nitrogen reduction reaction. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 23947-23954	13	15
65	Simulation of Phase-Change-Memory and Thermoelectric Materials using Machine-Learned Interatomic Potentials: Sb <sub>2</sub> Te <sub>3</sub> . <i>Physica Status Solidi (B): Basic Research</i> , <b>2020</b> , 258, 2000416	1.3	5
64	Temperature-induced structural change through the glass transition of silicate glass by neutron diffraction. <i>Physical Review B</i> , <b>2020</b> , 101,	3.3	4
63	Quantifying Chemical Structure and Machine-Learned Atomic Energies in Amorphous and Liquid Silicon. <i>Angewandte Chemie - International Edition</i> , <b>2019</b> , 58, 7057-7061	16.4	26
62	Quantifying Chemical Structure and Machine-Learned Atomic Energies in Amorphous and Liquid Silicon. <i>Angewandte Chemie</i> , <b>2019</b> , 131, 7131-7135	3.6	12
61	Mid-IR evanescent-field fiber sensor with enhanced sensitivity for volatile organic compounds.. <i>RSC Advances</i> , <b>2019</b> , 9, 21186-21191	3.7	5
60	Revealing the intrinsic nature of the mid-gap defects in amorphous GeSbTe. <i>Nature Communications</i> , <b>2019</b> , 10, 3065	17.4	51
59	Role of carbon-rings in polycrystalline GeSb <sub>2</sub> Te <sub>4</sub> phase-change material. <i>Journal of Alloys and Compounds</i> , <b>2019</b> , 782, 852-858	5.7	14
58	Gaussian approximation potential modeling of lithium intercalation in carbon nanostructures. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 241714	3.9	50
57	Small-angle x-ray scattering in amorphous silicon: A computational study. <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	8
56	Understanding the fast phase-change mechanism of tetrahedrally bonded Cu <sub>2</sub> GeTe <sub>3</sub> : Comprehensive analyses of electronic structure and transport phenomena. <i>Physical Review B</i> , <b>2018</b> , 97,	3.3	9
55	Understanding the thermal properties of amorphous solids using machine-learning-based interatomic potentials. <i>Molecular Simulation</i> , <b>2018</b> , 44, 866-880	2	47
54	Origin of radiation tolerance in amorphous GeSbTe phase-change random-access memory material. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2018</b> , 115, 5353-5358	11.5	16
53	Information-driven inverse approach to disordered solids: Applications to amorphous silicon. <i>Physical Review Materials</i> , <b>2018</b> , 2,	3.2	5
52	Ultrafast Nanoscale Phase-Change Memory Enabled By Single-Pulse Conditioning. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2018</b> , 10, 41855-41860	9.5	26

51	Computational Surface Chemistry of Tetrahedral Amorphous Carbon by Combining Machine Learning and Density Functional Theory. <i>Chemistry of Materials</i> , <b>2018</b> , 30, 7438-7445	9.6	48
50	Modeling the Phase-Change Memory Material, GeSbTe, with a Machine-Learned Interatomic Potential. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 8998-9006	3.4	62
49	Towards an atomistic understanding of disordered carbon electrode materials. <i>Chemical Communications</i> , <b>2018</b> , 54, 5988-5991	5.8	56
48	Realistic Atomistic Structure of Amorphous Silicon from Machine-Learning-Driven Molecular Dynamics. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 2879-2885	6.4	114
47	Similarity Between Amorphous and Crystalline Phases: The Case of TiO. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 2985-2990	6.4	49
46	The Relation between Chemical Bonding and Ultrafast Crystal Growth. <i>Advanced Materials</i> , <b>2017</b> , 29, 1700814	24	39
45	Morphology and Number Density of Voids in Hydrogenated Amorphous Silicon: An Ab Initio Study. <i>Physical Review Applied</i> , <b>2017</b> , 7,	4.3	13
44	First-principles simulations of vibrational decay and lifetimes in a-Si:H and a-Si:D. <i>Physical Review B</i> , <b>2017</b> , 95,	3.3	1
43	The significance of the amorphous potential energy landscape for dictating glassy dynamics and driving solid-state crystallisation. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 30039-30047	3.6	41
42	Structural properties of transition-metal clusters via force-biased Monte Carlo and ab initio calculations: A comparative study. <i>Physical Review B</i> , <b>2017</b> , 96,	3.3	4
41	Design of a Nanoscale, CMOS-Integrable, Thermal-Guiding Structure for Boolean-Logic and Neuromorphic Computation. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2016</b> , 8, 34530-34536	9.5	4
40	Metadynamical approach to the generation of amorphous structures: The case of a-Si:H. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	9
39	Analytical Capability of Defocused $\mu$ -SORS in the Chemical Interrogation of Thin Turbid Painted Layers. <i>Applied Spectroscopy</i> , <b>2016</b> , 70, 156-61	3.1	9
38	Estimation of semiconductor-like pigment concentrations in paint mixtures and their differentiation from paint layers using first-derivative reflectance spectra. <i>Talanta</i> , <b>2016</b> , 154, 63-72	6.2	9
37	Addendum and Erratum: Nature of vibrational excitations in vitreous silica [Phys. Rev. B 56, 8605 (1997)]. <i>Physical Review B</i> , <b>2016</b> , 94,	3.3	4
36	Chalcogenide Phase-Change Materials: Past and Future. <i>International Journal of Applied Glass Science</i> , <b>2015</b> , 6, 15-18	1.8	24
35	Ab Initio Molecular-Dynamics Simulation of Neuromorphic Computing in Phase-Change Memory Materials. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2015</b> , 7, 14223-30	9.5	22
34	A chemometric study of ageing in lead-based paints. <i>Talanta</i> , <b>2015</b> , 144, 977-85	6.2	5

33	Nanoscale structure of microvoids in a-Si:H: a first-principles study. <i>Journal of Physics Condensed Matter</i> , <b>2015</b> , 27, 435201	1.8	9
32	Microscopic Mechanism of Doping-Induced Kinetically Constrained Crystallization in Phase-Change Materials. <i>Advanced Materials</i> , <b>2015</b> , 27, 5477-83	24	49
31	n-type chalcogenides by ion implantation. <i>Nature Communications</i> , <b>2014</b> , 5, 5346	17.4	46
30	Thermal Decoupling of Molecular-Relaxation Processes from the Vibrational Density of States at Terahertz Frequencies in Supercooled Hydrogen-Bonded Liquids. <i>Journal of Physical Chemistry Letters</i> , <b>2014</b> , 5, 1968-72	6.4	49
29	Tailoring transient-amorphous states: towards fast and power-efficient phase-change memory and neuromorphic computing. <i>Advanced Materials</i> , <b>2014</b> , 26, 7493-8	24	51
28	Ultrafast phase-change logic device driven by melting processes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2014</b> , 111, 13272-7	11.5	48
27	Atomistic Origin of the Enhanced Crystallization Speed and n-Type Conductivity in Bi-doped Ge-Sb-Te Phase-Change Materials. <i>Advanced Functional Materials</i> , <b>2014</b> , 24, 7291-7300	15.6	28
26	Guest-cage atomic interactions in a clathrate-based phase-change material. <i>Advanced Materials</i> , <b>2014</b> , 26, 1725-30	24	3
25	Estimating the concentrations of pigments and binders in lead-based paints using FT-Raman spectroscopy and principal component analysis. <i>Journal of Raman Spectroscopy</i> , <b>2014</b> , 45, 1272-1278	2.3	10
24	Surfactant-free coating of thiols on gold nanoparticles using sonochemistry: a study of competing processes. <i>Ultrasonics Sonochemistry</i> , <b>2014</b> , 21, 1886-92	8.9	6
23	Interaction of metallic nanoparticles with dielectric substrates: effect of optical constants. <i>Nanotechnology</i> , <b>2013</b> , 24, 035201	3.4	41
22	Near-Field Plasmonics of an Individual Dielectric Nanoparticle above a Metallic Substrate. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 7784-7790	3.8	38
21	PCB-Integrated Optical Waveguide Sensors: An Ammonia Gas Sensor. <i>Journal of Lightwave Technology</i> , <b>2013</b> , 31, 1628-1635	4	13
20	Multivariate analysis of combined Raman and fibre-optic reflectance spectra for the identification of binder materials in simulated medieval paints. <i>Journal of Raman Spectroscopy</i> , <b>2013</b> , 44, 866-874	2.3	29
19	Near-field optical enhancement by lead-sulfide quantum dots and metallic nanoparticles for SERS. <i>Journal of Raman Spectroscopy</i> , <b>2013</b> , 44, 1292-1298	2.3	9
18	Preferred orientation of nanoscale order at the surface of amorphous Ge <sub>2</sub> Sb <sub>2</sub> Te <sub>5</sub> films. <i>Applied Physics Letters</i> , <b>2013</b> , 103, 201907	3.4	3
17	Metal oxide nanoparticle mediated enhanced Raman scattering and its use in direct monitoring of interfacial chemical reactions. <i>Nano Letters</i> , <b>2012</b> , 12, 4242-6	11.5	95
16	Formation of Spherical and Non-Spherical Eutectic Gallium-Indium Liquid-Metal Microdroplets in Microfluidic Channels at Room Temperature. <i>Advanced Functional Materials</i> , <b>2012</b> , 22, 2624-2631	15.6	86

15	Automated algorithm for baseline subtraction in spectra. <i>Journal of Raman Spectroscopy</i> , <b>2011</b> , 42, 363-369	2.9	28
14	Denoising of spectra with no user input: a spline-smoothing algorithm. <i>Journal of Raman Spectroscopy</i> , <b>2011</b> , 42, 370-376	2.3	11
13	Improved blind-source separation for spectra. <i>Journal of Raman Spectroscopy</i> , <b>2011</b> , 42, 1761-1768	2.3	7
12	Sensor Array Composed of Clicked Individual Microcantilever Chips. <i>Advanced Functional Materials</i> , <b>2011</b> , 21, 372-379	15.6	3
11	Atomic charge distribution in sodosilicate glasses from terahertz time-domain spectroscopy. <i>Physical Review B</i> , <b>2010</b> , 82,	3.3	21
10	Rapid prototyping of low-loss IR chalcogenide-glass waveguides by controlled remelting. <i>ChemPhysChem</i> , <b>2010</b> , 11, 2393-8	3.2	3
9	Simultaneous readout of multiple microcantilever arrays with phase-shifting interferometric microscopy. <i>Review of Scientific Instruments</i> , <b>2009</b> , 80, 093101	1.7	13
8	Computer Simulation of the Phase-change Cycle of GST-225. <i>Materials Research Society Symposia Proceedings</i> , <b>2008</b> , 1072, 1		0
7	Observation of light polarization-dependent structural changes in chalcogenide glasses. <i>Applied Physics Letters</i> , <b>2003</b> , 82, 706-708	3.4	38
6	Optical, electrical, and structural properties of amorphous Ag <sub>2</sub> TeS and Ag <sub>2</sub> TeSe films and comparison of photoinduced and thermally induced phenomena of both systems. <i>Journal of Applied Physics</i> , <b>1996</b> , 79, 9096-9104	2.5	77
5	Effect of addition of Au on the physical, electrical and optical properties of bulk glassy As <sub>2</sub> S <sub>3</sub> . <i>Journal of Applied Physics</i> , <b>1996</b> , 80, 5625-5632	2.5	4
4	Charge-transfer molecular dynamics. <i>The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties</i> , <b>1992</b> , 65, 489-500		43
3	Evaluation of Multiplexing in High-Density Holographic Memories		5
2	The Optomechanical Effect in Amorphous Chalcogenide Films		1
1	Study of Structural Changes in Glassy As <sub>2</sub> Se <sub>3</sub> by Exafs Under in-situ Laser Irradiation. <i>Ceramic Transactions</i> , 87-94	0.1	