Stephen R Elliott

List of Publications by Citations

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	Realistic Atomistic Structure of Amorphous Silicon from Machine-Learning-Driven Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2018**, 9, 2879-2885	6.4	114
85	Metal oxide nanoparticle mediated enhanced Raman scattering and its use in direct monitoring of interfacial chemical reactions. *Nano Letters*, **2012**, 12, 4242-6	11.5	95
84	Formation of Spherical and Non-Spherical Eutectic Gallium-Indium Liquid-Metal Microdroplets in Microfluidic Channels at Room Temperature. *Advanced Functional Materials*, **2012**, 22, 2624-2631	15.6	86
83	Optical, electrical, and structural properties of amorphous Ag□□e□ and Ag□□e□e films and comparison of photoinduced and thermally induced phenomena of both systems. *Journal of Applied Physics*, **1996**, 79, 9096-9104	2.5	77
82	Origins of structural and electronic transitions in disordered silicon. *Nature*, **2021**, 589, 59-64	50.4	66
81	Modeling the Phase-Change Memory Material, GeSbTe, with a Machine-Learned Interatomic Potential. *Journal of Physical Chemistry B*, **2018**, 122, 8998-9006	3.4	62
80	Towards an atomistic understanding of disordered carbon electrode materials. *Chemical Communications*, **2018**, 54, 5988-5991	5.8	56
79	Revealing the intrinsic nature of the mid-gap defects in amorphous GeSbTe. *Nature Communications*, **2019**, 10, 3065	17.4	51
78	Tailoring transient-amorphous states: towards fast and power-efficient phase-change memory and neuromorphic computing. *Advanced Materials*, **2014**, 26, 7493-8	24	51
77	Gaussian approximation potential modeling of lithium intercalation in carbon nanostructures. *Journal of Chemical Physics*, **2018**, 148, 241714	3.9	50
76	Thermal Decoupling of Molecular-Relaxation Processes from the Vibrational Density of States at Terahertz Frequencies in Supercooled Hydrogen-Bonded Liquids. *Journal of Physical Chemistry Letters*, **2014**, 5, 1968-72	6.4	49
75	Microscopic Mechanism of Doping-Induced Kinetically Constrained Crystallization in Phase-Change Materials. *Advanced Materials*, **2015**, 27, 5477-83	24	49
74	Similarity Between Amorphous and Crystalline□Phases: The□Case□of□TiO. *Journal of Physical Chemistry Letters*, **2018**, 9, 2985-2990	6.4	49
73	Ultrafast phase-change logic device driven by melting processes. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 13272-7	11.5	48
72	Computational Surface Chemistry of Tetrahedral Amorphous Carbon by Combining Machine Learning and Density Functional Theory. *Chemistry of Materials*, **2018**, 30, 7438-7445	9.6	48
71	Understanding the thermal properties of amorphous solids using machine-learning-based interatomic potentials. *Molecular Simulation*, **2018**, 44, 866-880	2	47
70	n-type chalcogenides by ion implantation. *Nature Communications*, **2014**, 5, 5346	17.4	46

69	Charge-transfer molecular dynamics. *The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties*, **1992**, 65, 489-500		43
68	The significance of the amorphous potential energy landscape for dictating glassy dynamics and driving solid-state crystallisation. *Physical Chemistry Chemical Physics*, **2017**, 19, 30039-30047	3.6	41
67	Interaction of metallic nanoparticles with dielectric substrates: effect of optical constants. *Nanotechnology*, **2013**, 24, 035201	3.4	41
66	The Relation between Chemical Bonding and Ultrafast Crystal Growth. *Advanced Materials*, **2017**, 29, 1700814	24	39
65	Near-Field Plasmonics of an Individual Dielectric Nanoparticle above a Metallic Substrate. *Journal of Physical Chemistry C*, **2013**, 117, 7784-7790	3.8	38
64	Observation of light polarization-dependent structural changes in chalcogenide glasses. *Applied Physics Letters*, **2003**, 82, 706-708	3.4	38
63	Multivariate analysis of combined Raman and fibre-optic reflectance spectra for the identification of binder materials in simulated medieval paints. *Journal of Raman Spectroscopy*, **2013**, 44, 866-874	2.3	29
62	Atomistic Origin of the Enhanced Crystallization Speed and n-Type Conductivity in Bi-doped Ge-Sb-Te Phase-Change Materials. *Advanced Functional Materials*, **2014**, 24, 7291-7300	15.6	28
61	Automated algorithm for baseline subtraction in spectra. *Journal of Raman Spectroscopy*, **2011**, 42, 363-369	2.3	28
60	Quantifying Chemical Structure and Machine-Learned Atomic Energies in Amorphous and Liquid Silicon. *Angewandte Chemie - International Edition*, **2019**, 58, 7057-7061	16.4	26
59	Ultrafast Nanoscale Phase-Change Memory Enabled By Single-Pulse Conditioning. *ACS Applied Materials & Interfaces*, **2018**, 10, 41855-41860	9.5	26
58	Chalcogenide Phase-Change Materials: Past and Future. *International Journal of Applied Glass Science*, **2015**, 6, 15-18	1.8	24
57	Ab Initio Molecular-Dynamics Simulation of Neuromorphic Computing in Phase-Change Memory Materials. *ACS Applied Materials & Interfaces*, **2015**, 7, 14223-30	9.5	22
56	Chemical Bonding in Chalcogenides: The Concept of Multicenter Hyperbonding. *Advanced Materials* , **2020**, 32, e2000340	24	21
55	Atomic charge distribution in sodosilicate glasses from terahertz time-domain spectroscopy. *Physical Review B*, **2010**, 82,	3.3	21
54	Synergy effect of co-doping Sc and Y in Sb2Te3 for phase-change memory. *Journal of Materials Chemistry C*, **2020**, 8, 6672-6679	7.1	16
53	Origin of radiation tolerance in amorphous GeSbTe phase-change random-access memory material. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 5353-5358	11.5	16
52	Two-dimensional molybdenum carbides: active electrocatalysts for the nitrogen reduction reaction. *Journal of Materials Chemistry A*, **2020**, 8, 23947-23954	13	15

51	Role of carbon-rings in polycrystalline GeSb2Te4 phase-change material. *Journal of Alloys and Compounds*, **2019**, 782, 852-858	5.7	14
50	Morphology and Number Density of Voids in Hydrogenated Amorphous Silicon: An Ab Initio Study. *Physical Review Applied*, **2017**, 7,	4.3	13
49	PCB-Integrated Optical Waveguide Sensors: An Ammonia Gas Sensor. *Journal of Lightwave Technology*, **2013**, 31, 1628-1635	4	13
48	Simultaneous readout of multiple microcantilever arrays with phase-shifting interferometric microscopy. *Review of Scientific Instruments*, **2009**, 80, 093101	1.7	13
47	Quantifying Chemical Structure and Machine-Learned Atomic Energies in Amorphous and Liquid Silicon. *Angewandte Chemie*, **2019**, 131, 7131-7135	3.6	12
46	Denoising of spectra with no user input: a spline-smoothing algorithm. *Journal of Raman Spectroscopy*, **2011**, 42, 370-376	2.3	11
45	Estimating the concentrations of pigments and binders in lead-based paints using FT-Raman spectroscopy and principal component analysis. *Journal of Raman Spectroscopy*, **2014**, 45, 1272-1278	2.3	10
44	Understanding the fast phase-change mechanism of tetrahedrally bonded Cu2GeTe3: Comprehensive analyses of electronic structure and transport phenomena. *Physical Review B*, **2018**, 97,	3.3	9
43	Metadynamical approach to the generation of amorphous structures: The case of a-Si:H. *Physical Review B*, **2016**, 93,	3.3	9
42	Analytical Capability of Defocused □-SORS in the Chemical Interrogation of Thin Turbid Painted Layers. *Applied Spectroscopy*, **2016**, 70, 156-61	3.1	9
41	Nanoscale structure of microvoids in a-Si:H: a first-principles study. *Journal of Physics Condensed Matter*, **2015**, 27, 435201	1.8	9
40	Near-field optical enhancement by lead-sulfide quantum dots and metallic nanoparticles for SERS. *Journal of Raman Spectroscopy*, **2013**, 44, 1292-1298	2.3	9
39	Estimation of semiconductor-like pigment concentrations in paint mixtures and their differentiation from paint layers using first-derivative reflectance spectra. *Talanta*, **2016**, 154, 63-72	6.2	9
38	Vacancy formation energy and its connection with bonding environment in solid: A high-throughput calculation and machine learning study. *Computational Materials Science*, **2020**, 183, 109803	3.2	8
37	Small-angle x-ray scattering in amorphous silicon: A computational study. *Physical Review B*, **2018**, 97,	3.3	8
36	Improved blind-source separation for spectra. *Journal of Raman Spectroscopy*, **2011**, 42, 1761-1768	2.3	7
35	ChemDataExtractor 2.0: Autopopulated Ontologies for Materials Science. *Journal of Chemical Information and Modeling*, **2021**, 61, 4280-4289	6.1	7
34	Surfactant-free coating of thiols on gold nanoparticles using sonochemistry: a study of competing processes. *Ultrasonics Sonochemistry*, **2014**, 21, 1886-92	8.9	6

33	On the Chemical Bonding of Amorphous Sb2Te3. *Physica Status Solidi - Rapid Research Letters*, **2021**, 15, 2000485	2.5	6
32	A chemometric study of ageing in lead-based paints. *Talanta*, **2015**, 144, 977-85	6.2	5
31	Mid-IR evanescent-field fiber sensor with enhanced sensitivity for volatile organic compounds.. *RSC Advances*, **2019**, 9, 21186-21191	3.7	5
30	Evaluation of Multiplexing in High-Density Holographic Memories338-356		5
29	Information-driven inverse approach to disordered solids: Applications to amorphous silicon. *Physical Review Materials*, **2018**, 2,	3.2	5
28	Simulation of Phase-Change-Memory and Thermoelectric Materials using Machine-Learned Interatomic Potentials: Sb2Te3. *Physica Status Solidi (B): Basic Research*, **2020**, 258, 2000416	1.3	5
27	Disorder by design: A data-driven approach to amorphous semiconductors without total-energy functionals. *Scientific Reports*, **2020**, 10, 7742	4.9	4
26	Design of a Nanoscale, CMOS-Integrable, Thermal-Guiding Structure for Boolean-Logic and Neuromorphic Computation. *ACS Applied Materials & Interfaces*, **2016**, 8, 34530-34536	9.5	4
25	Structural properties of transition-metal clusters via force-biased Monte Carlo and ab initio calculations: A comparative study. *Physical Review B*, **2017**, 96,	3.3	4
24	Effect of addition of Au on the physical, electrical and optical properties of bulk glassy As2S3. *Journal of Applied Physics*, **1996**, 80, 5625-5632	2.5	4
23	Real-time bioprocess monitoring using a mid-infrared fibre-optic sensor. *Biochemical Engineering Journal*, **2021**, 167, 107889	4.2	4
22	Addendum and Erratum: Nature of vibrational excitations in vitreous silica [Phys. Rev. B 56, 8605 (1997)]. *Physical Review B*, **2016**, 94,	3.3	4
21	Temperature-induced structural change through the glass transition of silicate glass by neutron diffraction. *Physical Review B*, **2020**, 101,	3.3	4
20	A fast, low-energy multi-state phase-change artificial synapse based on uniform partial-state transitions. *APL Materials*, **2021**, 9, 091103	5.7	4
19	Robust Design of High-Performance Optoelectronic Chalcogenide Crystals from High-Throughput Computation.. *Journal of the American Chemical Society*, **2022**,	16.4	4
18	Guest-cage atomic interactions in a clathrate-based phase-change material. *Advanced Materials*, **2014**, 26, 1725-30	24	3
17	Preferred orientation of nanoscale order at the surface of amorphous Ge2Sb2Te5 films. *Applied Physics Letters*, **2013**, 103, 201907	3.4	3
16	Sensor Array Composed of Clicked Individual Microcantilever Chips. *Advanced Functional Materials*, **2011**, 21, 372-379	15.6	3

15	Rapid prototyping of low-loss IR chalcogenide-glass waveguides by controlled remelting. *ChemPhysChem*, **2010**, 11, 2393-8	3.2	3
14	Multi-Center Hyperbonding in Phase-Change Materials. *Physica Status Solidi - Rapid Research Letters* , **2021**, 15, 2000516	2.5	3
13	Cerebral Microdialysate Metabolite Monitoring using Mid-infrared Spectroscopy. *Analytical Chemistry*, **2021**, 93, 11929-11936	7.8	3
12	Nonequilibrium ab initio molecular-dynamics simulations of lattice thermal conductivity in irradiated glassy Ge 2 Sb 2 Te 5. *Applied Physics Letters*, **2020**, 116, 031902	3.4	2
11	Antibonding-Induced Anomalous Temperature Dependence of the Band Gap in Crystalline Ge2Sb2Te5. *Journal of Physical Chemistry C*, **2021**, 125, 19537-19543	3.8	2
10	First-principles simulations of vibrational decay and lifetimes in a-Si:H and a-Si:D. *Physical Review B*, **2017**, 95,	3.3	1
9	The Optomechanical Effect in Amorphous Chalcogenide Films109-118		1
8	Electric-field-induced annihilation of localized gap defect states in amorphous phase-change memory materials. *Acta Materialia*, **2021**, 223, 117465	8.4	1
7	Temperature-induced nanostructural evolution of hydrogen-rich voids in amorphous silicon: a first-principles study. *Nanoscale*, **2020**, 12, 1464-1477	7.7	1
6	Novel metal oxides with promising high-temperature thermoelectric performance. *Journal of Materials Chemistry C*, **2021**, 9, 12884-12894	7.1	1
5	Elucidation of the Nature of Structural Relaxation in Glassy d-Sorbitol. *Journal of Physical Chemistry B*, **2020**, 124, 1833-1838	3.4	0
4	Computer Simulation of the Phase-change Cycle of GST-225. *Materials Research Society Symposia Proceedings*, **2008**, 1072, 1		0
3	Quasilocalized Vibrations in Vitreous Silica. *Physica Status Solidi (B): Basic Research*, **2020**, 258, 2000422	1.3	
2	Study of Structural Changes in Glassy As2Se3 by Exafs Under in-situ Laser Irradiation. *Ceramic Transactions*,87-94	0.1	
1	Crystallization of Phase-Change Chalcogenides **2021**, 367-402		