Jonathan M Skelton

List of Publications by Year in Descending Order

92 papers	3,406 citations	28 h-index	57 g-index
129 ext. papers	4,153 ext. citations	7.1 avg, IF	5.57 L-index

#	Paper	IF	Citations
92	Structural dynamics of Schottky and Frenkel defects in ThO2: a density-functional theory study. *Journal of Materials Chemistry A*, **2022**, 10, 1861-1875	13	1
91	Thermoelectric Properties of Pnma and Rocksalt SnS and SnSe. *Solids*, **2022**, 3, 155-176	0	0
90	Two Is Better than One? Investigating the Effect of Incorporating Re(CO)Cl Side Chains into Pt(II) Diynes and Polyynes. *Inorganic Chemistry*, **2021**, 60, 745-759	5.1	3
89	Impact of noble-gas filler atoms on the lattice thermal conductivity of CoSb3 skutterudites: first-principles modelling. *Journal of Physics Condensed Matter*, **2021**,	1.8	4
88	Bulk and Surface Conformations in Solid-State Lovastatin: Spectroscopic and Molecular Dynamics Studies. *Crystals*, **2021**, 11, 509	2.3	1
87	Synthesis, characterization, and optoelectronic properties of phenothiazine-based organic co-poly-ynes. *New Journal of Chemistry*, **2021**, 45, 15082-15095	3.6	1
86	Approximate models for the lattice thermal conductivity of alloy thermoelectrics. *Journal of Materials Chemistry C*, **2021**, 9, 11772-11787	7.1	4
85	Phase stability of the tin monochalcogenides SnS and SnSe: a quasi-harmonic lattice-dynamics study. *Physical Chemistry Chemical Physics*, **2021**, 23, 19219-19236	3.6	3
84	CaSbO and CaBiO: two promising mixed-anion thermoelectrics. *Journal of Materials Chemistry A*, **2021**, 9, 20417-20435	13	3
83	Use of Interplay between A-Site Non-Stoichiometry and Hydroxide Doping to Deliver Novel Proton-Conducting Perovskite Oxides. *Advanced Energy Materials*, **2021**, 11, 2101337	21.8	1
82	Unraveling the Impact of Graphene Addition to Thermoelectric SrTiO and La-Doped SrTiO Materials: A Density Functional Theory Study. *ACS Applied Materials & Interfaces*, **2021**, 13, 41303-41314	9.5	2
81	Understanding magnetic relaxation in single-ion magnets with high blocking temperature. *Physical Review B*, **2020**, 101,	3.3	41
80	Accuracy of Hybrid Functionals with Non-Self-Consistent Kohn-Sham Orbitals for Predicting the Properties of Semiconductors. *Journal of Chemical Theory and Computation*, **2020**, 16, 3543-3557	6.4	12
79	Polymorph exploration of bismuth stannate using first-principles phonon mode mapping.. *Chemical Science*, **2020**, 11, 7904-7909	9.4	2
78	Electronic and Phonon Instabilities in Bilayer Graphene under Applied External Bias. *Materials Today: Proceedings*, **2020**, 20, 373-382	1.4	1
77	Lattice dynamics of Pnma Sn(S1⊠ Se x) solid solutions: energetics, phonon spectra and thermal transport. *JPhys Energy*, **2020**, 2, 025006	4.9	3
76	Sn 5s2 lone pairs and the electronic structure of tin sulphides: A photoreflectance, high-energy photoemission, and theoretical investigation. *Physical Review Materials*, **2020**, 4,	3.2	4

75	Assessment of dynamic structural instabilities across 24 cubic inorganic halide perovskites. *Journal of Chemical Physics*, **2020**, 152, 024703	3.9	28
74	Bi2Sn2O7: a potential room temperature n-type oxide thermoelectric. *Journal of Materials Chemistry A*, **2020**, 8, 16405-16420	13	10
73	Chemical Trends in the Lattice Thermal Conductivity of Li(Ni, Mn, Co)O2 (NMC) Battery Cathodes. *Chemistry of Materials*, **2020**, 32, 7542-7550	9.6	14
72	Watching Photochemistry Happen: Recent Developments in Dynamic Single-Crystal X-Ray Diffraction Studies. *Structure and Bonding*, **2020**, 199-238	0.9	1
71	Highly Anisotropic Thermal Transport in LiCoO. *Journal of Physical Chemistry Letters*, **2019**, 10, 5552-5556	6.4	12
70	Experimental Evidence for Vibrational Entropy as Driving Parameter of Flexibility in the Metal Organic Framework ZIF-4(Zn). *Chemistry of Materials*, **2019**, 31, 8366-8372	9.6	18
69	Room Temperature Metallic Conductivity in a Metal-Organic Framework Induced by Oxidation. *Journal of the American Chemical Society*, **2019**, 141, 16323-16330	16.4	49
68	Thermodynamics, Electronic Structure, and Vibrational Properties of Sn (S Se) Solid Solutions for Energy Applications. *Chemistry of Materials*, **2019**, 31, 3672-3685	9.6	6
67	Intrinsic Flexibility of the EMT Zeolite Framework under Pressure. *Molecules*, **2019**, 24,	4.8	6
66	Photocrystallographic Studies on Transition Metal Nitrito Metastable Linkage Isomers: Manipulating the Metastable State. *Accounts of Chemical Research*, **2019**, 52, 1079-1088	24.3	24
65	Living in the salt-cocrystal continuum: indecisive organic complexes with thermochromic behaviour. *CrystEngComm*, **2019**, 21, 1626-1634	3.3	16
64	Lattice vibrations of and coronene from Raman microscopy and theory. *Physical Review Materials*, **2019**, 3,	3.2	3
63	SMACT: Semiconducting Materials by Analogy and Chemical Theory. *Journal of Open Source Software*, **2019**, 4, 1361	5.2	10
62	Shining Light on Growth-Dependent Surface Chemistry of Organic Crystals: A Polarized Raman Spectroscopic and Computational Study of Aspirin. *Crystal Growth and Design*, **2019**, 19, 1288-1298	3.5	3
61	Monitoring photo-induced population dynamics in metastable linkage isomer crystals: a crystallographic kinetic study of [Pd(Budien)NO]BPh. *Physical Chemistry Chemical Physics*, **2018**, 20, 5874-5886	3.6	15
60	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
59	Computer-aided design of metal chalcohalide semiconductors: from chemical composition to crystal structure. *Chemical Science*, **2018**, 9, 1022-1030	9.4	35
58	Acoustic phonon lifetimes limit thermal transport in methylammonium lead iodide. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 11905-11910	11.5	52

57	Ultrafast Nanoscale Phase-Change Memory Enabled By Single-Pulse Conditioning. *ACS Applied Materials & Interfaces*, **2018**, 10, 41855-41860	9.5	26
56	Hydrogen Bonding versus Entropy: Revealing the Underlying Thermodynamics of the Hybrid Organic□norganic Perovskite [CH3NH3]PbBr3. *Chemistry of Materials*, **2018**, 30, 8782-8788	9.6	19
55	Chemical and Lattice Stability of the Tin Sulfides. *Journal of Physical Chemistry C*, **2017**, 121, 6446-6454	3.8	52
54	Exploring Structure□Property Relationships of Silver 4-(Phenylethynyl)pyridine Complexes. *European Journal of Inorganic Chemistry*, **2017**, 2017, 1855-1867	2.3	4
53	Anion□□□nteractions and Metastability: Structural Transformations in a Silver□Pyrazine Network. *European Journal of Inorganic Chemistry*, **2017**, 2017, 2628-2636	2.3	4
52	Lattice dynamics of the tin sulphides SnS, SnS and SnS: vibrational spectra and thermal transport. *Physical Chemistry Chemical Physics*, **2017**, 19, 12452-12465	3.6	108
51	Metastable cubic tin sulfide: A novel phonon-stable chiral semiconductor. *APL Materials*, **2017**, 5, 036101	5.7	36
50	Spontaneous Octahedral Tilting in the Cubic Inorganic Cesium Halide Perovskites CsSnX and CsPbX (X = F, Cl, Br, I). *Journal of Physical Chemistry Letters*, **2017**, 8, 4720-4726	6.4	126
49	Electronic Structure of Transition-Metal Based Cu2GeTe3 Phase Change Material: Revealing the Key Role of Cu d Electrons. *Chemistry of Materials*, **2017**, 29, 7440-7449	9.6	18
48	A rapidly-reversible absorptive and emissive vapochromic Pt(II) pincer-based chemical sensor. *Nature Communications*, **2017**, 8, 1800	17.4	56
47	Low-frequency optical phonon modes and carrier mobility in the halide perovskite CH3NH3PbBr3 using terahertz time-domain spectroscopy. *Applied Physics Letters*, **2017**, 111, 201903	3.4	38
46	Metallic Conductivity in a Two-Dimensional Cobalt Dithiolene Metal-Organic Framework. *Journal of the American Chemical Society*, **2017**, 139, 10863-10867	16.4	209
45	Anharmonicity in the High-Temperature Cmcm Phase of SnSe: Soft Modes and Three-Phonon Interactions. *Physical Review Letters*, **2016**, 117, 075502	7.4	104
44	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
43	Computational Screening of All Stoichiometric Inorganic Materials. *CheM*, **2016**, 1, 617-627	16.2	72
42	Impact of the Alkyne Substitution Pattern and Metalation on the Photoisomerization of Azobenzene-Based Platinum(II) Diynes and Polyynes. *Inorganic Chemistry*, **2016**, 55, 10955-10967	5.1	16
41	A general forcefield for accurate phonon properties of metal-organic frameworks. *Physical Chemistry Chemical Physics*, **2016**, 18, 29316-29329	3.6	26
40	Experimental and Theoretical Investigation for the Level of Conjugation in Carbazole-Based Precursors and Their Mono-, Di-, and Polynuclear Pt(II) Complexes. *Inorganic Chemistry*, **2016**, 55, 6465-80	5.1	20

39	Dynamic disorder, phonon lifetimes, and the assignment of modes to the vibrational spectra of methylammonium lead halide perovskites. *Physical Chemistry Chemical Physics*, **2016**, 18, 27051-27066	3.6	243
38	Electronic and optical properties of single crystal SnS2: an earth-abundant disulfide photocatalyst. *Journal of Materials Chemistry A*, **2016**, 4, 1312-1318	13	190
37	Computational materials design of crystalline solids. *Chemical Society Reviews*, **2016**, 45, 6138-6146	58.5	72
36	Observation of a re-entrant phase transition in the molecular complex tris(□3,5-diiso-propyl-1,2,4-triazolato-□)trigold(I) under high pressure. *IUCrJ*, **2016**, 3, 367-376	4.7	5
35	Phonon anharmonicity, lifetimes, and thermal transport in CH3NH3PbI3 from many-body perturbation theory. *Physical Review B*, **2016**, 94,	3.3	101
34	Suppression of lattice thermal conductivity by mass-conserving cation mutation in multi-component semiconductors. *APL Materials*, **2016**, 4, 104809	5.7	8
33	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
32	Free Energy of Ligand Removal in the Metal-Organic Framework UiO-66. *Journal of Physical Chemistry C*, **2016**, 120, 9276-9281	3.8	34
31	Band Alignments, Valence Bands, and Core Levels in the Tin Sulfides SnS, SnS2, and Sn2S3: Experiment and Theory. *Chemistry of Materials*, **2016**, 28, 3718-3726	9.6	123
30	Direct Observation of Dynamic Symmetry Breaking above Room Temperature in Methylammonium Lead Iodide Perovskite. *ACS Energy Letters*, **2016**, 1, 880-887	20.1	177
29	Ab Initio Molecular-Dynamics Simulations of Doped Phase-Change Materials. *Springer Series in Materials Science*, **2015**, 441-456	0.9	
28	Ab Initio Molecular-Dynamics Simulation of Neuromorphic Computing in Phase-Change Memory Materials. *ACS Applied Materials & Interfaces*, **2015**, 7, 14223-30	9.5	22
27	Energetics, thermal isomerisation and photochemistry of the linkage-isomer system [Ni(Et4dien)(□2-O,ON)(□1-NO2)]. *CrystEngComm*, **2015**, 17, 383-394	3.3	12
26	A chemometric study of ageing in lead-based paints. *Talanta*, **2015**, 144, 977-85	6.2	5
25	Time and Space resolved Methods: general discussion. *Faraday Discussions*, **2015**, 177, 263-92	3.6	1
24	Vibrational spectra and lattice thermal conductivity of kesterite-structured Cu2ZnSnS4 and Cu2ZnSnSe4. *APL Materials*, **2015**, 3, 041102	5.7	55
23	Solid-state chemistry of glassy antimony oxides. *Journal of Materials Chemistry C*, **2015**, 3, 11349-11356	7.1	8
22	Electronic excitations in molecular solids: bridging theory and experiment. *Faraday Discussions*, **2015**, 177, 181-202	3.6	10

21	Sulfamerazine: Understanding the Influence of Slip Planes in the Polymorphic Phase Transformation through X-Ray Crystallographic Studies and ab Initio Lattice Dynamics. *Molecular Pharmaceutics*, **2015**, 12, 3735-48	5.6	8
20	Crystalline adducts of the Lawsone molecule (2-hydroxy-1,4-naphthaquinone): optical properties and computational modelling. *CrystEngComm*, **2015**, 17, 7684-7692	3.3	11
19	Phase stability and transformations in the halide perovskite CsSnI3. *Physical Review B*, **2015**, 91,	3.3	101
18	Lattice dynamics and vibrational spectra of the orthorhombic, tetragonal, and cubic phases of methylammonium lead iodide. *Physical Review B*, **2015**, 92,	3.3	360
17	Crystal structure optimisation using an auxiliary equation of state. *Journal of Chemical Physics*, **2015** , 143, 184101	3.9	15
16	Influence of the exchange-correlation functional on the quasi-harmonic lattice dynamics of II-VI semiconductors. *Journal of Chemical Physics*, **2015**, 143, 064710	3.9	60
15	Dynamics of chemical bond: general discussion. *Faraday Discussions*, **2015**, 177, 121-54	3.6	8
14	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
13	Thermal physics of the lead chalcogenides PbS, PbSe, and PbTe from first principles. *Physical Review B*, **2014**, 89,	3.3	172
12	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
11	A Raman spectroscopic study of uranyl minerals from Cornwall, UK. *RSC Advances*, **2014**, 4, 59137-59149	3.7	25
10	Guest-cage atomic interactions in a clathrate-based phase-change material. *Advanced Materials*, **2014**, 26, 1725-30	24	3
9	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
8	Surfactant-free coating of thiols on gold nanoparticles using sonochemistry: a study of competing processes. *Ultrasonics Sonochemistry*, **2014**, 21, 1886-92	8.9	6
7	Structural insights into the formation and evolution of amorphous phase-change materials. *Physica Status Solidi (B): Basic Research*, **2013**, 250, 968-975	1.3	12
6	In silico optimization of phase-change materials for digital memories: a survey of first-row transition-metal dopants for Ge□Sb□Te□ *Journal of Physics Condensed Matter*, **2013**, 25, 205801	1.8	15
5	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
4	Origin of the unusual reflectance and density contrasts in the phase-change material Cu2GeTe3. *Applied Physics Letters*, **2013**, 102, 224105	3.4	30

3	Understanding the multistate SET process in Ge-Sb-Te-based phase-change memory. *Journal of Applied Physics*, **2012**, 112, 064901	2.5	15
2	Structural, dynamical, and electronic properties of transition metal-doped Ge2Sb2Te5 phase-change materials simulated by ab initio molecular dynamics. *Applied Physics Letters*, **2012**, 101, 024106	3.4	15
1	Structural Dynamics and Thermal Transport in Bismuth Chalcogenide Alloys. *Chemistry of Materials*,	9.6	1