Jonathan M Skelton

List of Publications by Year
in descending order

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100 papers	4,928 citations	126708 33 h-index	95083 68 g-index
129 all docs	129 docs citations	129 times ranked	7406 citing authors

#	Article	IF	Citations
1	Lattice dynamics and vibrational spectra of the orthorhombic, tetragonal, and cubic phases of methylammonium lead iodide. Physical Review B, 2015, 92, .	1.1	452
2	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.	1.3	325
3	Metallic Conductivity in a Two-Dimensional Cobalt Dithiolene Metalâ€“Organic Framework. Journal of the American Chemical Society, 2017, 139, 10863-10867.	6.6	300
4	Electronic and optical properties of single crystal SnS₂: an earth-abundant disulfide photocatalyst. Journal of Materials Chemistry A, 2016, 4, 1312-1318.	5.2	246
5	Direct Observation of Dynamic Symmetry Breaking above Room Temperature in Methylammonium Lead Iodide Perovskite. ACS Energy Letters, 2016, 1, 880-887.	8.8	221
6	Thermal physics of the lead chalcogenides PbS, PbSe, and PbTe from first principles. Physical Review B, 2014, 89, .	1.1	212
7	Lattice dynamics of the tin sulphides SnS₂, SnS and Sn₂S₃: vibrational spectra and thermal transport. Physical Chemistry Chemical Physics, 2017, 19, 12452-12465.	1.3	187
8	Spontaneous Octahedral Tilting in the Cubic Inorganic Cesium Halide Perovskites CsSnX₃ and CsPbX₃ (X = F, Cl, Br, I). Journal of Physical Chemistry Letters, 2017, 8, 4720-4726.	2.1	186
9	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.	3.2	172
10	Anharmonicity in the High-Temperature<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>C</mml:mi><mml:mi>m</mml:mi><mml:mi>c</mml:mi><mml:mi>m</mml:mi></mml:math>Phase of SnSe: Soft Modes and Three-Phonon Interactions. Physical Review Letters, 2016, 117, 075502.	7.8	147
11	Phase stability and transformations in the halide perovskite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CsSnI</mml:mi><mml:mn>3</mml:mn></mml:msub><m Physical Review B, 2015, 91, .	1.1	138
12	Phonon anharmonicity, lifetimes, and thermal transport in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>CH</mml:mi><mml:mn>3</mml:mn></mml:msub></mml: from many-body perturbation theory. Physical Review B, 2016, 94, .	1.1	131
13	Computational Screening of All Stoichiometric Inorganic Materials. CheM, 2016, 1, 617-627.	5.8	115
14	Computational materials design of crystalline solids. Chemical Society Reviews, 2016, 45, 6138-6146.	18.7	105
15	Understanding magnetic relaxation in single-ion magnets with high blocking temperature. Physical Review B, 2020, 101, .	1.1	94
16	Room Temperature Metallic Conductivity in a Metalâ€“Organic Framework Induced by Oxidation. Journal of the American Chemical Society, 2019, 141, 16323-16330.	6.6	93
17	A rapidly-reversible absorptive and emissive vapochromic Pt(II) pincer-based chemical sensor. Nature Communications, 2017, 8, 1800.	5.8	83
18	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.	3.3	81

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19	Influence of the exchange-correlation functional on the quasi-harmonic lattice dynamics of II-VI semiconductors. Journal of Chemical Physics, 2015, 143, 064710.	1.2	80
20	Chemical and Lattice Stability of the Tin Sulfides. Journal of Physical Chemistry C, 2017, 121, 6446-6454.	1.5	73
21	Vibrational spectra and lattice thermal conductivity of kesterite-structured Cu2ZnSnS4 and Cu2ZnSnSe4. APL Materials, 2015, 3, .	2.2	69
22	Assessment of dynamic structural instabilities across 24 cubic inorganic halide perovskites. Journal of Chemical Physics, 2020, 152, 024703.	1.2	67
23	Ultrafast phase-change logic device driven by melting processes. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 13272-13277.	3.3	56
24	Low-frequency optical phonon modes and carrier mobility in the halide perovskite CH3NH3PbBr3 using terahertz time-domain spectroscopy. Applied Physics Letters, 2017, 111, .	1.5	54
25	Computer-aided design of metal chalcohalide semiconductors: from chemical composition to crystal structure. Chemical Science, 2018, 9, 1022-1030.	3.7	54
26	Metastable cubic tin sulfide: A novel phonon-stable chiral semiconductor. APL Materials, 2017, 5, 036101.	2.2	51
27	Free Energy of Ligand Removal in the Metalâ€“Organic Framework UiO-66. Journal of Physical Chemistry C, 2016, 120, 9276-9281.	1.5	46
28	The physical significance of imaginary phonon modes in crystals. Electronic Structure, 2022, 4, 033002.	1.0	41
29	A general forcefield for accurate phonon properties of metalâ€“organic frameworks. Physical Chemistry Chemical Physics, 2016, 18, 29316-29329.	1.3	40
30	Atomistic Origin of the Enhanced Crystallization Speed and nâ€Type Conductivity in Biâ€doped Geâ€Sbâ€Te Phaseâ€Change Materials. Advanced Functional Materials, 2014, 24, 7291-7300.	7.8	38
31	Photocrystallographic Studies on Transition Metal Nitrito Metastable Linkage Isomers: Manipulating the Metastable State. Accounts of Chemical Research, 2019, 52, 1079-1088.	7.6	38
32	Origin of the unusual reflectance and density contrasts in the phase-change material Cu₂GeTe₃. Applied Physics Letters, 2013, 102, 224105.	1.5	37
33	Ultrafast Nanoscale Phase-Change Memory Enabled By Single-Pulse Conditioning. ACS Applied Materials & Interfaces, 2018, 10, 41855-41860.	4.0	36
34	A Raman spectroscopic study of uranyl minerals from Cornwall, UK. RSC Advances, 2014, 4, 59137-59149.	1.7	33
35	Multivariate analysis of combined Raman and fibreâ€optic reflectance spectra for the identification of binder materials in simulated medieval paints. Journal of Raman Spectroscopy, 2013, 44, 866-874.	1.2	32
36	Hydrogen Bonding versus Entropy: Revealing the Underlying Thermodynamics of the Hybrid Organicâ€“Inorganic Perovskite [CH₃NH₃]PbBr₃. Chemistry of Materials, 2018, 30, 8782-8788.	3.2	29

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37	Experimental Evidence for Vibrational Entropy as Driving Parameter of Flexibility in the Metalâ€“Organic Framework ZIF-4(Zn). Chemistry of Materials, 2019, 31, 8366-8372.	3.2	29
38	Ab Initio Molecular-Dynamics Simulation of Neuromorphic Computing in Phase-Change Memory Materials. ACS Applied Materials & Interfaces, 2015, 7, 14223-14230.	4.0	28
39	Living in the salt-cocrystal continuum: indecisive organic complexes with thermochromic behaviour. CrystEngComm, 2019, 21, 1626-1634.	1.3	28
40	Chemical Trends in the Lattice Thermal Conductivity of Li(Ni, Mn, Co)O₂ (NMC) Battery Cathodes. Chemistry of Materials, 2020, 32, 7542-7550.	3.2	28
41	Monitoring photo-induced population dynamics in metastable linkage isomer crystals: a crystallographic kinetic study of [Pd(Bu₄dien)NO₂]BPh₄. Physical Chemistry Chemical Physics, 2018, 20, 5874-5886.	1.3	25
42	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, 6465-6480.	1.9	24
43	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.	3.2	24
44	Viewpoint: Atomic-Scale Design Protocols toward Energy, Electronic, Catalysis, and Sensing Applications. Inorganic Chemistry, 2019, 58, 14939-14980.	1.9	23
45	Ca₄Sb₂O and Ca₄Bi₂O: two promising mixed-anion thermoelectrics. Journal of Materials Chemistry A, 2021, 9, 20417-20435.	5.2	22
46	In silicooptimization of phase-change materials for digital memories: a survey of first-row transition-metal dopants for Ge₂Sb₂Te₅. Journal of Physics Condensed Matter, 2013, 25, 205801.	0.7	21
47	Crystal structure optimisation using an auxiliary equation of state. Journal of Chemical Physics, 2015, 143, 184101.	1.2	21
48	SMACT: Semiconducting Materials by Analogy and Chemical Theory. Journal of Open Source Software, 2019, 4, 1361.	2.0	21
49	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.	1.9	19
50	Structural, dynamical, and electronic properties of transition metal-doped Ge2Sb2Te5 phase-change materials simulated by ab initio molecular dynamics. Applied Physics Letters, 2012, 101, .	1.5	17
51	Highly Anisotropic Thermal Transport in LiCoO₂. Journal of Physical Chemistry Letters, 2019, 10, 5552-5556.	2.1	17
52	Î±-Bi₂Sn₂O₇: a potential room temperature n-type oxide thermoelectric. Journal of Materials Chemistry A, 2020, 8, 16405-16420.	5.2	17
53	Accuracy of Hybrid Functionals with Non-Self-Consistent Kohnâ€“Sham Orbitals for Predicting the Properties of Semiconductors. Journal of Chemical Theory and Computation, 2020, 16, 3543-3557.	2.3	17
54	Understanding the multistate SET process in Ge-Sb-Te-based phase-change memory. Journal of Applied Physics, 2012, 112, .	1.1	16

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55	Energetics, thermal isomerisation and photochemistry of the linkage-isomer system [Ni(Et₄dien)(Î·²-O,ON)(Î·¹-NO₂)]. CrystEngComm, 2015, 17, 383-394.	1.3	16
56	Structural insights into the formation and evolution of amorphous phaseâ€change materials. Physica Status Solidi (B): Basic Research, 2013, 250, 968-975.	0.7	15
57	Design of a Nanoscale, CMOS-Integrable, Thermal-Guiding Structure for Boolean-Logic and Neuromorphic Computation. ACS Applied Materials & Interfaces, 2016, 8, 34530-34536.	4.0	15
58	Ge 4s² lone pairs and band alignments in GeS and GeSe for photovoltaics. Journal of Materials Chemistry A, 2021, 9, 22440-22452.	5.2	15
59	Crystalline adducts of the Lawsone molecule (2-hydroxy-1,4-naphthaquinone): optical properties and computational modelling. CrystEngComm, 2015, 17, 7684-7692.	1.3	14
60	Phase stability of the tin monochalcogenides SnS and SnSe: a quasi-harmonic lattice-dynamics study. Physical Chemistry Chemical Physics, 2021, 23, 19219-19236.	1.3	14
61	Unraveling the Impact of Graphene Addition to Thermoelectric SrTiO₃ and La-Doped SrTiO₃ Materials: A Density Functional Theory Study. ACS Applied Materials & Interfaces, 2021, 13, 41303-41314.	4.0	14
62	Estimating the concentrations of pigments and binders in leadâ€based paints using FTâ€Raman spectroscopy and principal component analysis. Journal of Raman Spectroscopy, 2014, 45, 1272-1278.	1.2	12
63	Solid-state chemistry of glassy antimony oxides. Journal of Materials Chemistry C, 2015, 3, 11349-11356.	2.7	12
64	Suppression of lattice thermal conductivity by mass-conserving cation mutation in multi-component semiconductors. APL Materials, 2016, 4, 104809.	2.2	12
65	Approximate models for the lattice thermal conductivity of alloy thermoelectrics. Journal of Materials Chemistry C, 2021, 9, 11772-11787.	2.7	12
66	Y₂Ti₂O₅S₂ â€“ a promising n-type oxysulphide for thermoelectric applications. Journal of Materials Chemistry A, 2022, 10, 16813-16824.	5.2	12
67	Electronic excitations in molecular solids: bridging theory and experiment. Faraday Discussions, 2015, 177, 181-202.	1.6	11
68	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.	2.9	11
69	Understanding the fast phase-change mechanism of tetrahedrally bonded <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Cu</mml:mi><mml:mn>2</mml:mn></mml: : Comprehensive analyses of electronic structure and transport phenomena. Physical Review B, 2018, 97, .	1.1	11
70	Thermodynamics, Electronic Structure, and Vibrational Properties of Snn(S1â€“xSex)m Solid Solutions for Energy Applications. Chemistry of Materials, 2019, 31, 3672-3685.	3.2	11
71	Polymorph exploration of bismuth stannate using first-principles phonon mode mapping. Chemical Science, 2020, 11, 7904-7909.	3.7	11
72	Use of Interplay between Aâ€Site Nonâ€Stoichiometry and Hydroxide Doping to Deliver Novel Protonâ€Conducting Perovskite Oxides. Advanced Energy Materials, 2021, 11, 2101337.	10.2	11

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73	Sn 5s2 lone pairs and the electronic structure of tin sulphides: A photoreflectance, high-energy photoemission, and theoretical investigation. Physical Review Materials, 2020, 4, .	0.9	11
74	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, 3735-3748.	2.3	10
75	Structural Dynamics and Thermal Transport in Bismuth Chalcogenide Alloys. Chemistry of Materials, 2021, 33, 8404-8417.	3.2	10
76	Structural dynamics of Schottky and Frenkel defects in ThO₂: a density-functional theory study. Journal of Materials Chemistry A, 2022, 10, 1861-1875.	5.2	9
77	Surfactant-free coating of thiols on gold nanoparticles using sonochemistry: A study of competing processes. Ultrasonics Sonochemistry, 2014, 21, 1886-1892.	3.8	8
78	Dynamics of chemical bond: general discussion. Faraday Discussions, 2015, 177, 121-154.	1.6	8
79	Intrinsic Flexibility of the EMT Zeolite Framework under Pressure. Molecules, 2019, 24, 641.	1.7	8
80	Impact of noble-gas filler atoms on the lattice thermal conductivity of CoSb₃ skutterudites: first-principles modelling. Journal of Physics Condensed Matter, 2021, 33, 164002.	0.7	8
81	Two Is Better than One? Investigating the Effect of Incorporating Re(CO)3Cl Side Chains into Pt(II) Diynes and Polyynes. Inorganic Chemistry, 2021, 60, 745-759.	1.9	8
82	Thermoelectric Properties of Pnma and Rocksalt SnS and SnSe. Solids, 2022, 3, 155-176.	1.1	7
83	A chemometric study of ageing in lead-based paints. Talanta, 2015, 144, 977-985.	2.9	6
84	Exploring Structureâ€“Property Relationships of Silver 4â€(Phenylethynyl)pyridine Complexes. European Journal of Inorganic Chemistry, 2017, 2017, 1855-1867.	1.0	6
85	Observation of a re-entrant phase transition in the molecular complex tris(Î¼₂-3,5-diisopropyl-1,2,4-triazolato-Îº²N¹:N²)trigold(I) under high pressure. IUCrJ, 2016, 3, 367-376.	2.3	6
86	Guestâ€Cage Atomic Interactions in a Clathrateâ€Based Phaseâ€Change Material. Advanced Materials, 2014, 26, 1725-1730.	11.1	5
87	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.	1.4	5
88	AnionÂ·Â·Â·Ï€ Interactions and Metastability: Structural Transformations in a Silverâ€“Pyrazine Network. European Journal of Inorganic Chemistry, 2017, 2017, 2628-2636.	1.0	4
89	Electronic and Phonon Instabilities in Bilayer Graphene under Applied External Bias. Materials Today: Proceedings, 2020, 20, 373-382.	0.9	4
90	Lattice dynamics of Pnma Sn(S_{1â€“x}Se_x) solid solutions: energetics, phonon spectra and thermal transport. JPhys Energy, 2020, 2, 025006.	2.3	4

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91	Lattice vibrations ofÎ³- andÎ²-coronene from Raman microscopy and theory. Physical Review Materials, 2019, 3, .	0.9	4
92	Towards an atomistic understanding of polymorphism in molecular solids. Physical Chemistry Chemical Physics, 2022, 24, 11278-11294.	1.3	4
93	Synthesis, characterization, and optoelectronic properties of phenothiazine-based organic co-poly-ynes. New Journal of Chemistry, 2021, 45, 15082-15095.	1.4	3
94	Watching Photochemistry Happen: Recent Developments in Dynamic Single-Crystal X-Ray Diffraction Studies. Structure and Bonding, 2020, , 199-238.	1.0	2
95	Time and Space resolved Methods: general discussion. Faraday Discussions, 2015, 177, 263-292.	1.6	1
96	Bulk and Surface Conformations in Solid-State Lovastatin: Spectroscopic and Molecular Dynamics Studies. Crystals, 2021, 11, 509.	1.0	1
97	Ab Initio Molecular-Dynamics Simulations of Doped Phase-Change Materials. Springer Series in Materials Science, 2015, , 441-456.	0.4	0
98	Ab initio lattice dynamics for materials design and characterisation. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C77-C77.	0.0	0
99	10.1063/1.4917044.1. , 2015, , .		0
100	Watching chemistry happen â€“ dynamic studies of light-induced transformations in linkage isomerism complexes. Acta Crystallographica Section A: Foundations and Advances, 2018, 74, e123-e123.	0.0	0