

Keith T Butler

List of Publications by Year in descending order

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88
papers

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citations

101543

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93
docs citations

93
times ranked

13641
citing authors

#	ARTICLE	IF	CITATIONS
1	Origin of Ferroelectricity in Two Prototypical Hybrid Organic-Inorganic Perovskites. <i>Journal of the American Chemical Society</i> , 2022, 144, 816-823.	13.7	47
2	Breaking the Aristotype: Featurization of Polyhedral Distortions in Perovskite Crystals. <i>Chemistry of Materials</i> , 2022, 34, 562-573.	6.7	8
3	Ultralow work function of the electride Sr ₃ CrN ₃ . <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 8854-8858.	2.8	3
4	Mixed-anion mixed-cation perovskite (FAPb ₃) _{0.875} (MAPbBr ₃) _{0.125} : an <i>ab initio</i> molecular dynamics study. <i>Journal of Materials Chemistry A</i> , 2022, 10, 9592-9603.	10.3	4
5	Distributed representations of atoms and materials for machine learning. <i>Npj Computational Materials</i> , 2022, 8, .	8.7	9
6	Interpretable and Explainable Machine Learning for Materials Science and Chemistry. <i>Accounts of Materials Research</i> , 2022, 3, 597-607.	11.7	60
7	UnlockNN: Uncertainty quantification for neural network models of chemical systems. <i>Journal of Open Source Software</i> , 2022, 7, 3700.	4.6	2
8	Tilt and shift polymorphism in molecular perovskites. <i>Materials Horizons</i> , 2021, 8, 2444-2450.	12.2	12
9	Interpretable, calibrated neural networks for analysis and understanding of inelastic neutron scattering data. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 194006.	1.8	7
10	Revealing the Potential Crystal Structures of Earth-Abundant Nontoxic Photovoltaic CuBi ₄ . <i>Crystal Growth and Design</i> , 2021, 21, 2850-2855.	3.0	8
11	Quantum Statistical Transport Phenomena in Memristive Computing Architectures. <i>Physical Review Applied</i> , 2021, 15, .	3.8	2
12	A deep convolutional neural network for real-time full profile analysis of big powder diffraction data. <i>Npj Computational Materials</i> , 2021, 7, .	8.7	31
13	Bandgap Engineering in the Configurational Space of Solid Solutions via Machine Learning: (Mg,Zn)O Case Study. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 5163-5168.	4.6	8
14	Best practices in machine learning for chemistry. <i>Nature Chemistry</i> , 2021, 13, 505-508.	13.6	240
15	Cycling Rate-Induced Spatially-Resolved Heterogeneities in Commercial Cylindrical Li-Ion Batteries. <i>Small Methods</i> , 2021, 5, e2100512.	8.6	12
16	Entropy-based active learning of graph neural network surrogate models for materials properties. <i>Journal of Chemical Physics</i> , 2021, 155, 174116.	3.0	14
17	Revealing the crystal structures and relative dielectric constants of fluorinated silicon oxides. <i>Journal of Materials Chemistry C</i> , 2021, 9, 15983-15989.	5.5	3
18	Modeling the dielectric constants of crystals using machine learning. <i>Journal of Chemical Physics</i> , 2020, 153, 024503.	3.0	29

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19	Differentiating the role of organic additives to assemble open framework aluminosilicates using INS spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 14177-14186.	2.8	1
20	Machine learning and big scientific data. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2020, 378, 20190054.	3.4	43
21	Understanding the Balance of Entropy and Enthalpy in Hydrogenâ€“Halide Noncovalent Bonding. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3495-3500.	4.6	3
22	Understanding dynamic properties of materials using neutron spectroscopy and atomistic simulation. <i>Journal of Physics Communications</i> , 2020, 4, 072001.	1.2	21
23	Computers in neutron science. <i>Journal of Physics Communications</i> , 2020, 4, 110401.	1.2	1
24	Metal-free perovskites for non linear optical materials. <i>Chemical Science</i> , 2019, 10, 8187-8194.	7.4	46
25	Local Coordination in Metal-Organic Frameworks Probed in the Vibrational and Optical Regime by EELS. <i>Microscopy and Microanalysis</i> , 2019, 25, 606-607.	0.4	0
26	Data-Driven Discovery of Photoactive Quaternary Oxides Using First-Principles Machine Learning. <i>Chemistry of Materials</i> , 2019, 31, 7221-7230.	6.7	45
27	Experimental Evidence for Vibrational Entropy as Driving Parameter of Flexibility in the Metalâ€“Organic Framework ZIF-4(Zn). <i>Chemistry of Materials</i> , 2019, 31, 8366-8372.	6.7	29
28	Tuning the Negative Thermal Expansion Behavior of the Metalâ€“Organic Framework Cu ₃ BTC ₂ by Retrofitting. <i>Journal of the American Chemical Society</i> , 2019, 141, 10504-10509.	13.7	57
29	Quick-start guide for first-principles modelling of semiconductor interfaces. <i>JPhys Energy</i> , 2019, 1, 016001.	5.3	12
30	Designing interfaces in energy materials applications with first-principles calculations. <i>Npj Computational Materials</i> , 2019, 5, .	8.7	71
31	Finding a junction partner for candidate solar cell absorbers enargite and bournonite from electronic band and lattice matching. <i>Journal of Applied Physics</i> , 2019, 125, .	2.5	19
32	Accelerated optimization of transparent, amorphous zinc-tin-oxide thin films for optoelectronic applications. <i>APL Materials</i> , 2019, 7, .	5.1	23
33	SMACT: Semiconducting Materials by Analogy and Chemical Theory. <i>Journal of Open Source Software</i> , 2019, 4, 1361.	4.6	21
34	Materials discovery by chemical analogy: role of oxidation states in structure prediction. <i>Faraday Discussions</i> , 2018, 211, 553-568.	3.2	22
35	Band Engineering of Carbon Nitride Monolayers by N-Type, P-Type, and Isoelectronic Doping for Photocatalytic Applications. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 11143-11151.	8.0	92
36	Computer-aided design of metal chalcogenide semiconductors: from chemical composition to crystal structure. <i>Chemical Science</i> , 2018, 9, 1022-1030.	7.4	54

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37	Subwavelength Spatially Resolved Coordination Chemistry of Metal-Organic Framework Glass Blends. <i>Journal of the American Chemical Society</i> , 2018, 140, 17862-17866.	13.7	23
38	Hydrogen Bonding versus Entropy: Revealing the Underlying Thermodynamics of the Hybrid Organic-Inorganic Perovskite [CH ₃ NH ₃] ₃ PbBr ₃ . <i>Chemistry of Materials</i> , 2018, 30, 8782-8788.	6.7	29
39	The chemical forces underlying octahedral tilting in halide perovskites. <i>Journal of Materials Chemistry C</i> , 2018, 6, 12045-12051.	5.5	23
40	An Unusual Phase Transition Driven by Vibrational Entropy Changes in a Hybrid Organic-Inorganic Perovskite. <i>Angewandte Chemie</i> , 2018, 130, 9070-9074.	2.0	10
41	An Unusual Phase Transition Driven by Vibrational Entropy Changes in a Hybrid Organic-Inorganic Perovskite. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 8932-8936.	13.8	46
42	Machine learning for molecular and materials science. <i>Nature</i> , 2018, 559, 547-555.	27.8	2,387
43	Chemical bonding at the metal-organic framework/metal oxide interface: simulated epitaxial growth of MOF-5 on rutile TiO ₂ . <i>Journal of Materials Chemistry A</i> , 2017, 5, 6226-6232.	10.3	18
44	Designing porous electronic thin-film devices: band offsets and heteroepitaxy. <i>Faraday Discussions</i> , 2017, 201, 207-219.	3.2	36
45	Heterogeneous catalytic hydrogenation of CO ₂ by metal oxides: defect engineering - perfecting imperfection. <i>Chemical Society Reviews</i> , 2017, 46, 4631-4644.	38.1	304
46	Electroactive Nanoporous Metal Oxides and Chalcogenides by Chemical Design. <i>Chemistry of Materials</i> , 2017, 29, 3663-3670.	6.7	8
47	Theory of ionization potentials of nonmetallic solids. <i>Physical Review B</i> , 2017, 95, .	3.2	18
48	MOFs modeling and theory: general discussion. <i>Faraday Discussions</i> , 2017, 201, 233-245.	3.2	4
49	Electronic structure design for nanoporous, electrically conductive zeolitic imidazolate frameworks. <i>Journal of Materials Chemistry C</i> , 2017, 5, 7726-7731.	5.5	40
50	How Strong Is the Hydrogen Bond in Hybrid Perovskites?. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 6154-6159.	4.6	174
51	Halide Perovskite Heteroepitaxy: Bond Formation and Carrier Confinement at the Pb-CsPbBr ₃ Interface. <i>Journal of Physical Chemistry C</i> , 2017, 121, 27351-27356.	3.1	40
52	Quasi-particle electronic band structure and alignment of the V-VI-VII semiconductors SbSI, SbSBr, and SbSeI for solar cells. <i>Applied Physics Letters</i> , 2016, 108, .	3.3	59
53	Magnetic coupling in a hybrid Mn(acetylene dicarboxylate). <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 33329-33334.	2.8	4
54	Ultrafast carrier dynamics in BiVO ₄ : Interplay between free carriers, trapped carriers and low-frequency lattice vibrations. , 2016, , .		1

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55	Chemical principles for electroactive metal-organic frameworks. <i>MRS Bulletin</i> , 2016, 41, 870-876.	3.5	42
56	Computational Screening of All Stoichiometric Inorganic Materials. <i>CheM</i> , 2016, 1, 617-627.	11.7	115
57	Organised chaos: entropy in hybrid inorganic-organic systems and other materials. <i>Chemical Science</i> , 2016, 7, 6316-6324.	7.4	62
58	Analysis of electrostatic stability and ordering in quaternary perovskite solid solutions. <i>Physical Review B</i> , 2016, 93, .	3.2	10
59	Microscopic origin of entropy-driven polymorphism in hybrid organic-inorganic perovskite materials. <i>Physical Review B</i> , 2016, 94, .	3.2	48
60	Realistic Surface Descriptions of Heterometallic Interfaces: The Case of TiWC Coated in Noble Metals. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4475-4482.	4.6	24
61	The effect of bean origin and temperature on grinding roasted coffee. <i>Scientific Reports</i> , 2016, 6, 24483.	3.3	31
62	Lone-Pair Stabilization in Transparent Amorphous Tin Oxides: A Potential Route to p-Type Conduction Pathways. <i>Chemistry of Materials</i> , 2016, 28, 4706-4713.	6.7	33
63	Relativistic electronic structure and band alignment of BiSI and BiSeI: candidate photovoltaic materials. <i>Journal of Materials Chemistry A</i> , 2016, 4, 2060-2068.	10.3	127
64	Role of Amine-Cavity Interactions in Determining the Structure and Mechanical Properties of the Ferroelectric Hybrid Perovskite $[\text{NH}_3\text{NH}_2]\text{Zn}(\text{HCOO})_3$. <i>Chemistry of Materials</i> , 2016, 28, 312-317.	6.7	55
65	Computational materials design of crystalline solids. <i>Chemical Society Reviews</i> , 2016, 45, 6138-6146.	38.1	105
66	Interplay of Orbital and Relativistic Effects in Bismuth Oxyhalides: BiOF, BiOCl, BiOBr, and BiOI. <i>Chemistry of Materials</i> , 2016, 28, 1980-1984.	6.7	291
67	Screening procedure for structurally and electronically matched contact layers for high-performance solar cells: hybrid perovskites. <i>Journal of Materials Chemistry C</i> , 2016, 4, 1149-1158.	5.5	45
68	Crystal structure optimisation using an auxiliary equation of state. <i>Journal of Chemical Physics</i> , 2015, 143, 184101.	3.0	21
69	A tunable amorphous p-type ternary oxide system: The highly mismatched alloy of copper tin oxide. <i>Journal of Applied Physics</i> , 2015, 118, 105702.	2.5	5
70	Band energy control of molybdenum oxide by surface hydration. <i>Applied Physics Letters</i> , 2015, 107, .	3.3	26
71	Morphological control of band offsets for transparent bipolar heterojunctions: The Ådeker diode. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2015, 212, 1461-1465.	1.8	10
72	Polymorph Engineering of TiO_2 : Demonstrating How Absolute Reference Potentials Are Determined by Local Coordination. <i>Chemistry of Materials</i> , 2015, 27, 3844-3851.	6.7	113

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73	Lattice-mismatched heteroepitaxy of IV-VI thin films on PbTe(001): An ab initio study. <i>Physical Review B</i> , 2015, 91, .	3.2	7
74	Role of entropic effects in controlling the polymorphism in formate ABX_3 metal-organic frameworks. <i>Chemical Communications</i> , 2015, 51, 15538-15541.	4.1	66
75	Assessment of Hybrid Organic-Inorganic Antimony Sulfides for Earth-Abundant Photovoltaic Applications. <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 5009-5014.	4.6	47
76	Ferroelectric materials for solar energy conversion: photoferroics revisited. <i>Energy and Environmental Science</i> , 2015, 8, 838-848.	30.8	333
77	Band alignment of the hybrid halide perovskites $CH_3NH_3PbCl_3$, $CH_3NH_3PbBr_3$ and $CH_3NH_3PbI_3$. <i>Materials Horizons</i> , 2015, 2, 228-231.	12.2	238
78	Electronic Structure Modulation of Metal-Organic Frameworks for Hybrid Devices. <i>ACS Applied Materials & Interfaces</i> , 2014, 6, 22044-22050.	8.0	75
79	Electronic Chemical Potentials of Porous Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2014, 136, 2703-2706.	13.7	262
80	Crystal electron binding energy and surface work function control of tin dioxide. <i>Physical Review B</i> , 2014, 89, .	3.2	48
81	Atomistic Origins of High-Performance in Hybrid Halide Perovskite Solar Cells. <i>Nano Letters</i> , 2014, 14, 2584-2590.	9.1	2,068
82	Prediction of Electron Energies in Metal Oxides. <i>Accounts of Chemical Research</i> , 2014, 47, 364-372.	15.6	107
83	Molecular ferroelectric contributions to anomalous hysteresis in hybrid perovskite solar cells. <i>APL Materials</i> , 2014, 2, .	5.1	481
84	A computational investigation of nickel (silicides) as potential contact layers for silicon photovoltaic cells. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 395003.	1.8	10
85	Stoichiometrically graded SiN_x for improved surface passivation in high performance solar cells. <i>Journal of Applied Physics</i> , 2012, 112, .	2.5	7
86	Structural and electronic properties of silver/silicon interfaces and implications for solar cell performance. <i>Physical Review B</i> , 2011, 83, .	3.2	32
87	Molecular dynamics studies of the bonding properties of amorphous silicon nitride coatings on crystalline silicon. <i>Journal of Applied Physics</i> , 2011, 110, .	2.5	14
88	Machine Learning Approaches for Accelerating the Discovery of Thermoelectric Materials. <i>ACS Symposium Series</i> , 0, , 1-32.	0.5	5