Keith T Butler

List of Publications by Year
in descending order

88	9,253	101543	51608
papers	citations	36	86
		h-index	g-index

93	93	93	13641
all docs	docs citations	times ranked	citing authors

#	ARTICLE	IF	CITATIONS
1	Machine learning for molecular and materials science. Nature, 2018, 559, 547-555.	27.8	2,387
2	Atomistic Origins of High-Performance in Hybrid Halide Perovskite Solar Cells. Nano Letters, 2014, 14, 2584-2590.	9.1	2,068
3	Molecular ferroelectric contributions to anomalous hysteresis in hybrid perovskite solar cells. APL Materials, 2014, 2, .	5.1	481
4	Ferroelectric materials for solar energy conversion: photoferroics revisited. Energy and Environmental Science, 2015, 8, 838-848.	30.8	333
5	Heterogeneous catalytic hydrogenation of CO_2 by metal oxides: defect engineering â€" perfecting imperfection. Chemical Society Reviews, 2017, 46, 4631-4644.	38.1	304
6	Interplay of Orbital and Relativistic Effects in Bismuth Oxyhalides: BiOF, BiOCl, BiOBr, and BiOI. Chemistry of Materials, 2016, 28, 1980-1984.	6.7	291
7	Electronic Chemical Potentials of Porous Metalâ€"Organic Frameworks. Journal of the American Chemical Society, 2014, 136, 2703-2706.	13.7	262
8	Best practices in machine learning for chemistry. Nature Chemistry, 2021, 13, 505-508.	13.6	240
9	Band alignment of the hybrid halide perovskites $CH_3NH_3PbCl_3$, $CH_3NH_3PbBr_3$ and $CH_3NH_3PbI_3$. Materials Horizons, 2015, 2, 228-231.	12.2	238
10	How Strong Is the Hydrogen Bond in Hybrid Perovskites?. Journal of Physical Chemistry Letters, 2017, 8, 6154-6159.	4.6	174
11	Relativistic electronic structure and band alignment of BiSI and BiSeI: candidate photovoltaic materials. Journal of Materials Chemistry A, 2016, 4, 2060-2068.	10.3	127
12	Computational Screening of All Stoichiometric Inorganic Materials. CheM, 2016, 1, 617-627.	11.7	115
13	Polymorph Engineering of TiO_2: Demonstrating How Absolute Reference Potentials Are Determined by Local Coordination. Chemistry of Materials, 2015, 27, 3844-3851.	6.7	113
14	Prediction of Electron Energies in Metal Oxides. Accounts of Chemical Research, 2014, 47, 364-372.	15.6	107
15	Computational materials design of crystalline solids. Chemical Society Reviews, 2016, 45, 6138-6146.	38.1	105
16	Band Engineering of Carbon Nitride Monolayers by N-Type, P-Type, and Isoelectronic Doping for Photocatalytic Applications. ACS Applied Materials & Interfaces, 2018, 10, 11143-11151.	8.0	92
17	Electronic Structure Modulation of Metalâ€"Organic Frameworks for Hybrid Devices. ACS Applied Materials & Interfaces, 2014, 6, 22044-22050.	8.0	75
18	Designing interfaces in energy materials applications with first-principles calculations. Npj Computational Materials, 2019, 5, .	8.7	71

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19	Role of entropic effects in controlling the polymorphism in formate ABX$_3$ metal–organic frameworks. Chemical Communications, 2015, 51, 15538-15541.	4.1	66
20	Organised chaos: entropy in hybrid inorganic–organic systems and other materials. Chemical Science, 2016, 7, 6316-6324.	7.4	62
21	Interpretable and Explainable Machine Learning for Materials Science and Chemistry. Accounts of Materials Research, 2022, 3, 597-607.	11.7	60
22	Quasi-particle electronic band structure and alignment of the V-VI-VII semiconductors SbSI, SbSBr, and SbSeI for solar cells. Applied Physics Letters, 2016, 108, .	3.3	59
23	Tuning the Negative Thermal Expansion Behavior of the Metal–Organic Framework Cu$_3$BTC$_2$ by Retrofitting. Journal of the American Chemical Society, 2019, 141, 10504-10509.	13.7	57
24	Role of Amine–Cavity Interactions in Determining the Structure and Mechanical Properties of the Ferroelectric Hybrid Perovskite [NH$_3$NH$_2$]Zn(HCOO)$_3$. Chemistry of Materials, 2016, 28, 312-317.	6.7	55
25	Computer-aided design of metal chalcohalide semiconductors: from chemical composition to crystal structure. Chemical Science, 2018, 9, 1022-1030.	7.4	54
26	Crystal electron binding energy and surface work function control of tin dioxide. Physical Review B, 2014, 89, .	3.2	48
27	Microscopic origin of entropy-driven polymorphism in hybrid organic-inorganic perovskite materials. Physical Review B, 2016, 94, .	3.2	48
28	Assessment of Hybrid Organic–Inorganic Antimony Sulfides for Earth-Abundant Photovoltaic Applications. Journal of Physical Chemistry Letters, 2015, 6, 5009-5014.	4.6	47
29	Origin of Ferroelectricity in Two Prototypical Hybrid Organic–Inorganic Perovskites. Journal of the American Chemical Society, 2022, 144, 816-823.	13.7	47
30	An Unusual Phase Transition Driven by Vibrational Entropy Changes in a Hybrid Organic–Inorganic Perovskite. Angewandte Chemie - International Edition, 2018, 57, 8932-8936.	13.8	46
31	Metal-free perovskites for non linear optical materials. Chemical Science, 2019, 10, 8187-8194.	7.4	46
32	Screening procedure for structurally and electronically matched contact layers for high-performance solar cells: hybrid perovskites. Journal of Materials Chemistry C, 2016, 4, 1149-1158.	5.5	45
33	Data-Driven Discovery of Photoactive Quaternary Oxides Using First-Principles Machine Learning. Chemistry of Materials, 2019, 31, 7221-7230.	6.7	45
34	Machine learning and big scientific data. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2020, 378, 20190054.	3.4	43
35	Chemical principles for electroactive metal–organic frameworks. MRS Bulletin, 2016, 41, 870-876.	3.5	42
36	Electronic structure design for nanoporous, electrically conductive zeolitic imidazolate frameworks. Journal of Materials Chemistry C, 2017, 5, 7726-7731.	5.5	40

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37	Halide Perovskite Heteroepitaxy: Bond Formation and Carrier Confinement at the PbS–CsPbBr$_3$ Interface. Journal of Physical Chemistry C, 2017, 121, 27351-27356.	3.1	40
38	Designing porous electronic thin-film devices: band offsets and heteroepitaxy. Faraday Discussions, 2017, 201, 207-219.	3.2	36
39	Lone-Pair Stabilization in Transparent Amorphous Tin Oxides: A Potential Route to p-Type Conduction Pathways. Chemistry of Materials, 2016, 28, 4706-4713.	6.7	33
40	Structural and electronic properties of silver/silicon interfaces and implications for solar cell performance. Physical Review B, 2011, 83, .	3.2	32
41	The effect of bean origin and temperature on grinding roasted coffee. Scientific Reports, 2016, 6, 24483.	3.3	31
42	A deep convolutional neural network for real-time full profile analysis of big powder diffraction data. Npj Computational Materials, 2021, 7, .	8.7	31
43	Hydrogen Bonding versus Entropy: Revealing the Underlying Thermodynamics of the Hybrid Organic–Inorganic Perovskite [CH$_3$NH$_3$]PbBr$_3$. Chemistry of Materials, 2018, 30, 8782-8788.	6.7	29
44	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.	6.7	29
45	Modeling the dielectric constants of crystals using machine learning. Journal of Chemical Physics, 2020, 153, 024503.	3.0	29
46	Band energy control of molybdenum oxide by surface hydration. Applied Physics Letters, 2015, 107, .	3.3	26
47	Realistic Surface Descriptions of Heterometallic Interfaces: The Case of TiWC Coated in Noble Metals. Journal of Physical Chemistry Letters, 2016, 7, 4475-4482.	4.6	24
48	Subwavelength Spatially Resolved Coordination Chemistry of Metal–Organic Framework Glass Blends. Journal of the American Chemical Society, 2018, 140, 17862-17866.	13.7	23
49	The chemical forces underlying octahedral tilting in halide perovskites. Journal of Materials Chemistry C, 2018, 6, 12045-12051.	5.5	23
50	Accelerated optimization of transparent, amorphous zinc-tin-oxide thin films for optoelectronic applications. APL Materials, 2019, 7, .	5.1	23
51	Materials discovery by chemical analogy: role of oxidation states in structure prediction. Faraday Discussions, 2018, 211, 553-568.	3.2	22
52	Crystal structure optimisation using an auxiliary equation of state. Journal of Chemical Physics, 2015, 143, 184101.	3.0	21
53	Understanding dynamic properties of materials using neutron spectroscopy and atomistic simulation. Journal of Physics Communications, 2020, 4, 072001.	1.2	21
54	SMACT: Semiconducting Materials by Analogy and Chemical Theory. Journal of Open Source Software, 2019, 4, 1361.	4.6	21

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55	Finding a junction partner for candidate solar cell absorbers enargite and bournonite from electronic band and lattice matching. Journal of Applied Physics, 2019, 125, .	2.5	19
56	Chemical bonding at the metal–organic framework/metal oxide interface: simulated epitaxial growth of MOF-5 on rutile TiO_2. Journal of Materials Chemistry A, 2017, 5, 6226-6232.	10.3	18
57	Theory of ionization potentials of nonmetallic solids. Physical Review B, 2017, 95, .	3.2	18
58	Molecular dynamics studies of the bonding properties of amorphous silicon nitride coatings on crystalline silicon. Journal of Applied Physics, 2011, 110, .	2.5	14
59	Entropy-based active learning of graph neural network surrogate models for materials properties. Journal of Chemical Physics, 2021, 155, 174116.	3.0	14
60	Quick-start guide for first-principles modelling of semiconductor interfaces. JPhys Energy, 2019, 1, 016001.	5.3	12
61	Tilt and shift polymorphism in molecular perovskites. Materials Horizons, 2021, 8, 2444-2450.	12.2	12
62	Cycling Rate–Induced Spatially–Resolved Heterogeneities in Commercial Cylindrical Li–Ion Batteries. Small Methods, 2021, 5, e2100512.	8.6	12
63	A computational investigation of nickel (silicides) as potential contact layers for silicon photovoltaic cells. Journal of Physics Condensed Matter, 2013, 25, 395003.	1.8	10
64	Morphological control of band offsets for transparent bipolar heterojunctions: The Bädeker diode. Physica Status Solidi (A) Applications and Materials Science, 2015, 212, 1461-1465.	1.8	10
65	Analysis of electrostatic stability and ordering in quaternary perovskite solid solutions. Physical Review B, 2016, 93, .	3.2	10
66	An Unusual Phase Transition Driven by Vibrational Entropy Changes in a Hybrid Organic–Inorganic Perovskite. Angewandte Chemie, 2018, 130, 9070-9074.	2.0	10
67	Distributed representations of atoms and materials for machine learning. Npj Computational Materials, 2022, 8, .	8.7	9
68	Electroactive Nanoporous Metal Oxides and Chalcogenides by Chemical Design. Chemistry of Materials, 2017, 29, 3663-3670.	6.7	8
69	Revealing the Potential Crystal Structures of Earth-Abundant Nontoxic Photovoltaic $CuBiI_4$. Crystal Growth and Design, 2021, 21, 2850-2855.	3.0	8
70	Bandgap Engineering in the Configurational Space of Solid Solutions via Machine Learning: (Mg,Zn)O Case Study. Journal of Physical Chemistry Letters, 2021, 12, 5163-5168.	4.6	8
71	Breaking the Aristotype: Featurization of Polyhedral Distortions in Perovskite Crystals. Chemistry of Materials, 2022, 34, 562-573.	6.7	8
72	Stoichiometrically graded SiN_x for improved surface passivation in high performance solar cells. Journal of Applied Physics, 2012, 112, .	2.5	7

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73	Lattice-mismatched heteroepitaxy of IV-VI thin films on PbTe(001): Anab initiostudy. Physical Review B, 2015, 91, .	3.2	7
74	Interpretable, calibrated neural networks for analysis and understanding of inelastic neutron scattering data. Journal of Physics Condensed Matter, 2021, 33, 194006.	1.8	7
75	A tunable amorphous p-type ternary oxide system: The highly mismatched alloy of copper tin oxide. Journal of Applied Physics, 2015, 118, 105702.	2.5	5
76	Machine Learning Approaches for Accelerating the Discovery of Thermoelectric Materials. ACS Symposium Series, 0, , 1-32.	0.5	5
77	Magnetic coupling in a hybrid Mn(ii) acetylene dicarboxylate. Physical Chemistry Chemical Physics, 2016, 18, 33329-33334.	2.8	4
78	MOFs modeling and theory: general discussion. Faraday Discussions, 2017, 201, 233-245.	3.2	4
79	Mixed-anion mixed-cation perovskite $(FAPbI_3)_{0.875}(MAPbBr_3)_{0.125}$: an *ab initio* molecular dynamics study. Journal of Materials Chemistry A, 2022, 10, 9592-9603.	10.3	4
80	Understanding the Balance of Entropy and Enthalpy in Hydrogen–Halide Noncovalent Bonding. Journal of Physical Chemistry Letters, 2020, 11, 3495-3500.	4.6	3
81	Revealing the crystal structures and relative dielectric constants of fluorinated silicon oxides. Journal of Materials Chemistry C, 2021, 9, 15983-15989.	5.5	3
82	Ultralow work function of the electride Sr_3CrN_3. Physical Chemistry Chemical Physics, 2022, 24, 8854-8858.	2.8	3
83	Quantum Statistical Transport Phenomena in Memristive Computing Architectures. Physical Review Applied, 2021, 15, .	3.8	2
84	UnlockNN: Uncertainty quantification for neural network models of chemical systems. Journal of Open Source Software, 2022, 7, 3700.	4.6	2
85	Ultrafast carrier dynamics in $BiVO_4$: Interplay between free carriers, trapped carriers and low-frequency lattice vibrations. , 2016, , .		1
86	Differentiating the role of organic additives to assemble open framework aluminosilicates using INS spectroscopy. Physical Chemistry Chemical Physics, 2020, 22, 14177-14186.	2.8	1
87	Computers in neutron science. Journal of Physics Communications, 2020, 4, 110401.	1.2	1
88	Local Coordination in Metal-Organic Frameworks Probed in the Vibrational and Optical Regime by EELS. Microscopy and Microanalysis, 2019, 25, 606-607.	0.4	0