Keith T Butler

List of Publications by Year
in descending order

88 papers	9,253 citations	116194 36 h-index	58552 86 g-index
93 all docs	93 docs citations	93 times ranked	15905 citing authors

#	Article	IF	Citations
1	Origin of Ferroelectricity in Two Prototypical Hybrid Organicâ€“Inorganic Perovskites. Journal of the American Chemical Society, 2022, 144, 816-823.	6.6	47
2	Breaking the Aristotype: Featurization of Polyhedral Distortions in Perovskite Crystals. Chemistry of Materials, 2022, 34, 562-573.	3.2	8
3	Ultralow work function of the electride Sr₃CrN₃. Physical Chemistry Chemical Physics, 2022, 24, 8854-8858.	1.3	3
4	Mixed-anion mixed-cation perovskite (FAPbI₃)_{0.875}(MAPbBr₃)_{0.125}: an ab initio molecular dynamics study. Journal of Materials Chemistry A, 2022, 10, 9592-9603.	5.2	4
5	Distributed representations of atoms and materials for machine learning. Npj Computational Materials, 2022, 8, .	3.5	9
6	Interpretable and Explainable Machine Learning for Materials Science and Chemistry. Accounts of Materials Research, 2022, 3, 597-607.	5.9	60
7	UnlockNN: Uncertainty quantification for neural network models of chemical systems. Journal of Open Source Software, 2022, 7, 3700.	2.0	2
8	Tilt and shift polymorphism in molecular perovskites. Materials Horizons, 2021, 8, 2444-2450.	6.4	12
9	Interpretable, calibrated neural networks for analysis and understanding of inelastic neutron scattering data. Journal of Physics Condensed Matter, 2021, 33, 194006.	0.7	7
10	Revealing the Potential Crystal Structures of Earth-Abundant Nontoxic Photovoltaic CuBiI₄. Crystal Growth and Design, 2021, 21, 2850-2855.	1.4	8
11	Quantum Statistical Transport Phenomena in Memristive Computing Architectures. Physical Review Applied, 2021, 15, .	1.5	2
12	A deep convolutional neural network for real-time full profile analysis of big powder diffraction data. Npj Computational Materials, 2021, 7, .	3.5	31
13	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.	2.1	8
14	Best practices in machine learning for chemistry. Nature Chemistry, 2021, 13, 505-508.	6.6	240
15	Cycling Rateâ€Induced Spatiallyâ€Resolved Heterogeneities in Commercial Cylindrical Liâ€Ion Batteries. Small Methods, 2021, 5, e2100512.	4.6	12
16	Entropy-based active learning of graph neural network surrogate models for materials properties. Journal of Chemical Physics, 2021, 155, 174116.	1.2	14
17	Revealing the crystal structures and relative dielectric constants of fluorinated silicon oxides. Journal of Materials Chemistry C, 2021, 9, 15983-15989.	2.7	3
18	Modeling the dielectric constants of crystals using machine learning. Journal of Chemical Physics, 2020, 153, 024503.	1.2	29

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19	Differentiating the role of organic additives to assemble open framework aluminosilicates using INS spectroscopy. Physical Chemistry Chemical Physics, 2020, 22, 14177-14186.	1.3	1
20	Machine learning and big scientific data. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2020, 378, 20190054.	1.6	43
21	Understanding the Balance of Entropy and Enthalpy in Hydrogenâ€“Halide Noncovalent Bonding. Journal of Physical Chemistry Letters, 2020, 11, 3495-3500.	2.1	3
22	Understanding dynamic properties of materials using neutron spectroscopy and atomistic simulation. Journal of Physics Communications, 2020, 4, 072001.	0.5	21
23	Computers in neutron science. Journal of Physics Communications, 2020, 4, 110401.	0.5	1
24	Metal-free perovskites for non linear optical materials. Chemical Science, 2019, 10, 8187-8194.	3.7	46
25	Local Coordination in Metal-Organic Frameworks Probed in the Vibrational and Optical Regime by EELS. Microscopy and Microanalysis, 2019, 25, 606-607.	0.2	0
26	Data-Driven Discovery of Photoactive Quaternary Oxides Using First-Principles Machine Learning. Chemistry of Materials, 2019, 31, 7221-7230.	3.2	45
27	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
28	Tuning the Negative Thermal Expansion Behavior of the Metalâ€“Organic Framework Cu₃BTC₂ by Retrofitting. Journal of the American Chemical Society, 2019, 141, 10504-10509.	6.6	57
29	Quick-start guide for first-principles modelling of semiconductor interfaces. JPhys Energy, 2019, 1, 016001.	2.3	12
30	Designing interfaces in energy materials applications with first-principles calculations. Npj Computational Materials, 2019, 5, .	3.5	71
31	Finding a junction partner for candidate solar cell absorbers enargite and bournonite from electronic band and lattice matching. Journal of Applied Physics, 2019, 125, .	1.1	19
32	Accelerated optimization of transparent, amorphous zinc-tin-oxide thin films for optoelectronic applications. APL Materials, 2019, 7, .	2.2	23
33	SMACT: Semiconducting Materials by Analogy and Chemical Theory. Journal of Open Source Software, 2019, 4, 1361.	2.0	21
34	Materials discovery by chemical analogy: role of oxidation states in structure prediction. Faraday Discussions, 2018, 211, 553-568.	1.6	22
35	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.	4.0	92
36	Computer-aided design of metal chalcohalide semiconductors: from chemical composition to crystal structure. Chemical Science, 2018, 9, 1022-1030.	3.7	54

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37	Subwavelength Spatially Resolved Coordination Chemistry of Metalâ€“Organic Framework Glass Blends. Journal of the American Chemical Society, 2018, 140, 17862-17866.	6.6	23
38	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
39	The chemical forces underlying octahedral tilting in halide perovskites. Journal of Materials Chemistry C, 2018, 6, 12045-12051.	2.7	23
40	An Unusual Phase Transition Driven by Vibrational Entropy Changes in a Hybrid Organicâ€“Inorganic Perovskite. Angewandte Chemie, 2018, 130, 9070-9074.	1.6	10
41	An Unusual Phase Transition Driven by Vibrational Entropy Changes in a Hybrid Organicâ€“Inorganic Perovskite. Angewandte Chemie - International Edition, 2018, 57, 8932-8936.	7.2	46
42	Machine learning for molecular and materials science. Nature, 2018, 559, 547-555.	13.7	2,387
43	Chemical bonding at the metalâ€“organic framework/metal oxide interface: simulated epitaxial growth of MOF-5 on rutile TiO₂. Journal of Materials Chemistry A, 2017, 5, 6226-6232.	5.2	18
44	Designing porous electronic thin-film devices: band offsets and heteroepitaxy. Faraday Discussions, 2017, 201, 207-219.	1.6	36
45	Heterogeneous catalytic hydrogenation of CO₂by metal oxides: defect engineering â€“ perfecting imperfection. Chemical Society Reviews, 2017, 46, 4631-4644.	18.7	304
46	Electroactive Nanoporous Metal Oxides and Chalcogenides by Chemical Design. Chemistry of Materials, 2017, 29, 3663-3670.	3.2	8
47	Theory of ionization potentials of nonmetallic solids. Physical Review B, 2017, 95, .	1.1	18
48	MOFs modeling and theory: general discussion. Faraday Discussions, 2017, 201, 233-245.	1.6	4
49	Electronic structure design for nanoporous, electrically conductive zeolitic imidazolate frameworks. Journal of Materials Chemistry C, 2017, 5, 7726-7731.	2.7	40
50	How Strong Is the Hydrogen Bond in Hybrid Perovskites?. Journal of Physical Chemistry Letters, 2017, 8, 6154-6159.	2.1	174
51	Halide Perovskite Heteroepitaxy: Bond Formation and Carrier Confinement at the PbSâ€“CsPbBr₃ Interface. Journal of Physical Chemistry C, 2017, 121, 27351-27356.	1.5	40
52	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, .	1.5	59
53	Magnetic coupling in a hybrid Mn(<scp>ii</scp>) acetylene dicarboxylate. Physical Chemistry Chemical Physics, 2016, 18, 33329-33334.	1.3	4
54	Ultrafast carrier dynamics in BiVO<inf>4</inf>: Interplay between free carriers, trapped carriers and low-frequency lattice vibrations. , 2016, , .		1

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55	Chemical principles for electroactive metalâ€“organic frameworks. MRS Bulletin, 2016, 41, 870-876.	1.7	42
56	Computational Screening of All Stoichiometric Inorganic Materials. CheM, 2016, 1, 617-627.	5.8	115
57	Organised chaos: entropy in hybrid inorganicâ€“organic systems and other materials. Chemical Science, 2016, 7, 6316-6324.	3.7	62
58	Analysis of electrostatic stability and ordering in quaternary perovskite solid solutions. Physical Review B, 2016, 93, .	1.1	10
59	Microscopic origin of entropy-driven polymorphism in hybrid organic-inorganic perovskite materials. Physical Review B, 2016, 94, .	1.1	48
60	Realistic Surface Descriptions of Heterometallic Interfaces: The Case of TiWC Coated in Noble Metals. Journal of Physical Chemistry Letters, 2016, 7, 4475-4482.	2.1	24
61	The effect of bean origin and temperature on grinding roasted coffee. Scientific Reports, 2016, 6, 24483.	1.6	31
62	Lone-Pair Stabilization in Transparent Amorphous Tin Oxides: A Potential Route to p-Type Conduction Pathways. Chemistry of Materials, 2016, 28, 4706-4713.	3.2	33
63	Relativistic electronic structure and band alignment of BiSI and BiSeI: candidate photovoltaic materials. Journal of Materials Chemistry A, 2016, 4, 2060-2068.	5.2	127
64	Role of Amineâ€“Cavity Interactions in Determining the Structure and Mechanical Properties of the Ferroelectric Hybrid Perovskite [NH₃NH₂]Zn(HCOO)₃. Chemistry of Materials, 2016, 28, 312-317.	3.2	55
65	Computational materials design of crystalline solids. Chemical Society Reviews, 2016, 45, 6138-6146.	18.7	105
66	Interplay of Orbital and Relativistic Effects in Bismuth Oxyhalides: BiOF, BiOCl, BiOBr, and BiOI. Chemistry of Materials, 2016, 28, 1980-1984.	3.2	291
67	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.	2.7	45
68	Crystal structure optimisation using an auxiliary equation of state. Journal of Chemical Physics, 2015, 143, 184101.	1.2	21
69	A tunable amorphous p-type ternary oxide system: The highly mismatched alloy of copper tin oxide. Journal of Applied Physics, 2015, 118, 105702.	1.1	5
70	Band energy control of molybdenum oxide by surface hydration. Applied Physics Letters, 2015, 107, .	1.5	26
71	Morphological control of band offsets for transparent bipolar heterojunctions: The BÃdeker diode. Physica Status Solidi (A) Applications and Materials Science, 2015, 212, 1461-1465.	0.8	10
72	Polymorph Engineering of TiO₂: Demonstrating How Absolute Reference Potentials Are Determined by Local Coordination. Chemistry of Materials, 2015, 27, 3844-3851.	3.2	113

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73	Lattice-mismatched heteroepitaxy of IV-VI thin films on PbTe(001): Anab initiostudy. Physical Review B, 2015, 91, .	1.1	7
74	Role of entropic effects in controlling the polymorphism in formate ABX₃ metalâ€“organic frameworks. Chemical Communications, 2015, 51, 15538-15541.	2.2	66
75	Assessment of Hybrid Organicâ€“Inorganic Antimony Sulfides for Earth-Abundant Photovoltaic Applications. Journal of Physical Chemistry Letters, 2015, 6, 5009-5014.	2.1	47
76	Ferroelectric materials for solar energy conversion: photoferroics revisited. Energy and Environmental Science, 2015, 8, 838-848.	15.6	333
77	Band alignment of the hybrid halide perovskites CH₃NH₃PbCl₃, CH₃NH₃PbBr₃and CH₃NH₃PbI₃. Materials Horizons, 2015, 2, 228-231.	6.4	238
78	Electronic Structure Modulation of Metalâ€“Organic Frameworks for Hybrid Devices. ACS Applied Materials & Interfaces, 2014, 6, 22044-22050.	4.0	75
79	Electronic Chemical Potentials of Porous Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2014, 136, 2703-2706.	6.6	262
80	Crystal electron binding energy and surface work function control of tin dioxide. Physical Review B, 2014, 89, .	1.1	48
81	Atomistic Origins of High-Performance in Hybrid Halide Perovskite Solar Cells. Nano Letters, 2014, 14, 2584-2590.	4.5	2,068
82	Prediction of Electron Energies in Metal Oxides. Accounts of Chemical Research, 2014, 47, 364-372.	7.6	107
83	Molecular ferroelectric contributions to anomalous hysteresis in hybrid perovskite solar cells. APL Materials, 2014, 2, .	2.2	481
84	A computational investigation of nickel (silicides) as potential contact layers for silicon photovoltaic cells. Journal of Physics Condensed Matter, 2013, 25, 395003.	0.7	10
85	Stoichiometrically graded SiNx for improved surface passivation in high performance solar cells. Journal of Applied Physics, 2012, 112, .	1.1	7
86	Structural and electronic properties of silver/silicon interfaces and implications for solar cell performance. Physical Review B, 2011, 83, .	1.1	32
87	Molecular dynamics studies of the bonding properties of amorphous silicon nitride coatings on crystalline silicon. Journal of Applied Physics, 2011, 110, .	1.1	14
88	Machine Learning Approaches for Accelerating the Discovery of Thermoelectric Materials. ACS Symposium Series, 0, , 1-32.	0.5	5