John Buckeridge

List of Publications by Citations

50 papers	3,133 citations	24 h-index	53 g-index
53 ext. papers	3,562 ext. citations	6.1 avg, IF	5.14 L-index

#	Paper	IF	Citations
50	Band alignment of rutile and anatase TiO□*Nature Materials*, **2013**, 12, 798-801	27	1656
49	Anharmonicity in the High-Temperature Cmcm Phase of SnSe: Soft Modes and Three-Phonon Interactions. *Physical Review Letters*, **2016**, 117, 075502	7.4	104
48	Vibronic Structure in Room Temperature Photoluminescence of the Halide Perovskite CsBiBr. *Inorganic Chemistry*, **2017**, 56, 42-45	5.1	95
47	Polymorph Engineering of TiO2: Demonstrating How Absolute Reference Potentials Are Determined by Local Coordination. *Chemistry of Materials*, **2015**, 27, 3844-3851	9.6	92
46	Oxidation states and ionicity. *Nature Materials*, **2018**, 17, 958-964	27	91
45	Defects and Oxide Ion Migration in the Solid Oxide Fuel Cell Cathode Material LaFeO3. *Chemistry of Materials*, **2016**, 28, 8210-8220	9.6	79
44	Growth and properties of GaSbBi alloys. *Applied Physics Letters*, **2013**, 103, 142106	3.4	78
43	Determination of the nitrogen vacancy as a shallow compensating center in GaN doped with divalent metals. *Physical Review Letters*, **2015**, 114, 016405	7.4	58
42	Automated procedure to determine the thermodynamic stability of a material and the range of chemical potentials necessary for its formation relative to competing phases and compounds. *Computer Physics Communications*, **2014**, 185, 330-338	4.2	58
41	Electron Counting in Solids: Oxidation States, Partial Charges, and Ionicity. *Journal of Physical Chemistry Letters*, **2017**, 8, 2074-2075	6.4	50
40	Enhanced Photocatalytic and Antibacterial Ability of Cu-Doped Anatase TiO Thin Films: Theory and Experiment. *ACS Applied Materials & Interfaces*, **2020**, 12, 15348-15361	9.5	49
39	Engineering Valence Band Dispersion for High Mobility p-Type Semiconductors. *Chemistry of Materials*, **2017**, 29, 2402-2413	9.6	47
38	Deep vs shallow nature of oxygen vacancies and consequent n-type carrier concentrations in transparent conducting oxides. *Physical Review Materials*, **2018**, 2,	3.2	46
37	Understanding doping anomalies in degenerate p-type semiconductor LaCuOSe. *Journal of Materials Chemistry C*, **2014**, 2, 3429-3438	7.1	45
36	Limits to Doping of Wide Band Gap Semiconductors. *Chemistry of Materials*, **2013**, 25, 2924-2926	9.6	45
35	Crystal electron binding energy and surface work function control of tin dioxide. *Physical Review B*, **2014**, 89,	3.3	42
34	Defect Engineering of Earth-Abundant Solar Absorbers BiSI and BiSeI. *Chemistry of Materials*, **2018**, 30, 3827-3835	9.6	39

33	Dynamical response and instability in ceria under lattice expansion. *Physical Review B*, **2013**, 87,	3.3	38
32	Screening Divalent Metals for A- and B-Site Dopants in LaFeO3. *Chemistry of Materials*, **2017**, 29, 8147-8157	9.6	37
31	Bulk electronic, elastic, structural, and dielectric properties of the Weyl semimetal TaAs. *Physical Review B*, **2016**, 93,	3.3	33
30	Donor and acceptor characteristics of native point defects in GaN. *Journal Physics D: Applied Physics* , **2019**, 52, 335104	3	28
29	Defect formation in In2O3 and SnO2: a new atomistic approach based on accurate lattice energies. *Journal of Materials Chemistry C*, **2018**, 6, 12386-12395	7.1	28
28	Morphological Features and Band Bending at Nonpolar Surfaces of ZnO. *Journal of Physical Chemistry C*, **2015**, 119, 11598-11611	3.8	27
27	Identifying Raman modes of Sb2Se3 and their symmetries using angle-resolved polarised Raman spectra. *Journal of Materials Chemistry A*, **2020**, 8, 8337-8344	13	25
26	Band energy control of molybdenum oxide by surface hydration. *Applied Physics Letters*, **2015**, 107, 231605	3.4	23
25	Equilibrium point defect and charge carrier concentrations in a material determined through calculation of the self-consistent Fermi energy. *Computer Physics Communications*, **2019**, 244, 329-342	4.2	22
24	Nitrogen composition dependence of electron effective mass in GaAs1−xNx. *Physical Review B*, **2010**, 82,	3.3	18
23	Nonstoichiometry and Weyl fermionic behavior in TaAs. *Physical Review B*, **2016**, 94,	3.3	16
22	Prediction of multiband luminescence due to the gallium vacancy–oxygen defect complex in GaN. *Applied Physics Letters*, **2018**, 112, 262104	3.4	15
21	Efficient and accurate approach to modeling the microstructure and defect properties of LaCoO3. *Physical Review B*, **2016**, 93,	3.3	13
20	Dispelling the Myth of Passivated Codoping in TiO. *Chemistry of Materials*, **2019**, 31, 2577-2589	9.6	12
19	N incorporation and associated localized vibrational modes in GaSb. *Physical Review B*, **2014**, 89,	3.3	12
18	Thermodynamically accessible titanium clusters Ti, N = 2-32. *Physical Chemistry Chemical Physics*, **2018**, 20, 13962-13973	3.6	10
17	Double bubbles: a new structural motif for enhanced electron-hole separation in solids. *Physical Chemistry Chemical Physics*, **2014**, 16, 21098-105	3.6	10
16	From Stable ZnO and GaN Clusters to Novel Double Bubbles and Frameworks. *Inorganics*, **2014**, 2, 248-263	3.9	10

15	Single Step Solution Processed GaAs Thin Films from GaMe3 and tBuAsH2 under Ambient Pressure. *Journal of Physical Chemistry C*, **2016**, 120, 7013-7019	3.8	10
14	Demonstration of the donor characteristics of Si and O defects in GaN using hybrid QM/MM. *Physica Status Solidi (A) Applications and Materials Science*, **2017**, 214, 1600445	1.6	9
13	Band gap reduction in InNxSb1-x alloys: Optical absorption, k □P modeling, and density functional theory. *Applied Physics Letters*, **2016**, 109, 132104	3.4	9
12	Intrinsic point defects and the n- and p-type dopability of the narrow gap semiconductors GaSb and InSb. *Physical Review B*, **2019**, 100,	3.3	8
11	Electronic band structure and optical properties of boron arsenide. *Physical Review Materials*, **2019**, 3,	3.2	8
10	Mobility in gated GaNxAs1□ heterostructures as a probe of nitrogen-related electronic states. *Physical Review B*, **2011**, 84,	3.3	7
9	Heterostructures of GaN with SiC and ZnO enhance carrier stability and separation in framework semiconductors. *Physica Status Solidi (A) Applications and Materials Science*, **2017**, 214, 1600440	1.6	6
8	One-dimensional embedded cluster approach to modeling CdS nanowires. *Journal of Chemical Physics*, **2013**, 139, 124101	3.9	6
7	Buckeridge et□al. Reply. *Physical Review Letters*, **2015**, 115, 029702	7.4	5
6	Quantum Mechanical/Molecular Mechanical (QM/MM) Approaches **2017**, 647-680		3
5	Vibrational mode shifts as a measure of local strain in the dilute nitride semiconductor alloy GaNxAs1□. *Physical Review B*, **2009**, 79,	3.3	3
4	Vibrational signature of the Si□N defect in Si-doped GaNxAs1□. *Solid State Communications*, **2010**, 150, 1967-1970	1.6	3
3	BaBi2O6: A Promising n-Type Thermoelectric Oxide with the PbSb2O6 Crystal Structure. *Chemistry of Materials*, **2021**, 33, 7441-7456	9.6	2
2	One-Dimensional Nanosystems. *Series in Materials Science and Engineering*, **2016**, 47-81		1
1	The Interplay of Interstitial and Substitutional Copper in Zinc Oxide.. *Frontiers in Chemistry*, **2021**, 9, 780935	5	0