Aron Walsh

List of Publications by Year
in descending order

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416 papers	56,015 citations	1461 110 h-index	1446 226 g-index
483 all docs	483 docs citations	483 times ranked	50435 citing authors

#	Article	IF	Citations
1	Nanocrystals of Cesium Lead Halide Perovskites (CsPbX₃, X = Cl, Br, and I): Novel Optoelectronic Materials Showing Bright Emission with Wide Color Gamut. Nano Letters, 2015, 15, 3692-3696.	4.5	6,814
2	Machine learning for molecular and materials science. Nature, 2018, 559, 547-555.	13.7	2,387
3	Ionic transport in hybrid lead iodide perovskite solar cells. Nature Communications, 2015, 6, 7497.	5.8	2,154
4	Atomistic Origins of High-Performance in Hybrid Halide Perovskite Solar Cells. Nano Letters, 2014, 14, 2584-2590.	4.5	2,068
5	Band alignment of rutile and anatase TiO2. Nature Materials, 2013, 12, 798-801.	13.3	1,924
6	Classification of Lattice Defects in the Kesterite Cu₂ZnSnS₄ and Cu₂ZnSnSe₄ Earthâ€Abundant Solar Cell Absorbers. Advanced Materials, 2013, 25, 1522-1539.	11.1	1,210
7	Consensus statement for stability assessment and reporting for perovskite photovoltaics based on ISOS procedures. Nature Energy, 2020, 5, 35-49.	19.8	797
8	Engineering the Optical Response of the Titanium-MIL-125 Metalâ€“Organic Framework through Ligand Functionalization. Journal of the American Chemical Society, 2013, 135, 10942-10945.	6.6	701
9	Band Edge Electronic Structure of BiVO₄: Elucidating the Role of the Bi s and V d Orbitals. Chemistry of Materials, 2009, 21, 547-551.	3.2	624
10	Intrinsic point defects and complexes in the quaternary kesterite semiconductor<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Cu</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu Physical Review B, 2010, 81, .	1.1	624
11	Relativistic quasiparticle self-consistent electronic structure of hybrid halide perovskite photovoltaic absorbers. Physical Review B, 2014, 89, .	1.1	612
12	Stereochemistry of post-transition metal oxides: revision of the classical lone pair model. Chemical Society Reviews, 2011, 40, 4455.	18.7	590
13	Kesterite Thinâ€Film Solar Cells: Advances in Materials Modelling of Cu₂ZnSnS₄. Advanced Energy Materials, 2012, 2, 400-409.	10.2	589
14	Crystal and electronic band structure of Cu2ZnSnX4 (X=S and Se) photovoltaic absorbers: First-principles insights. Applied Physics Letters, 2009, 94, .	1.5	585
15	Nature of the Band Gap of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>In</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>Revealed by First-Principles Calculations and X-Ray Spectroscopy. Physical Review Letters, 2008, 100, 167402.	2.9	576
16	Structural and electronic properties of hybrid perovskites for high-efficiency thin-film photovoltaics from first-principles. APL Materials, 2013, 1, .	2.2	517
17	The dynamics of methylammonium ions in hybrid organicâ€“inorganic perovskite solar cells. Nature Communications, 2015, 6, 7124.	5.8	517
18	Selfâ€Regulation Mechanism for Charged Point Defects in Hybrid Halide Perovskites. Angewandte Chemie - International Edition, 2015, 54, 1791-1794.	7.2	484

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19	Molecular ferroelectric contributions to anomalous hysteresis in hybrid perovskite solar cells. APL Materials, 2014, 2, .	2.2	481
20	Cubic Perovskite Structure of Black Formamidinium Lead Iodide, Î±-[HC(NH₂)₂]PbI₃, at 298 K. Journal of Physical Chemistry Letters, 2015, 6, 3209-3212.	2.1	457
21	Defect physics of the kesterite thin-film solar cell absorber Cu2ZnSnS4. Applied Physics Letters, 2010, 96, .	1.5	454
22	Lattice dynamics and vibrational spectra of the orthorhombic, tetragonal, and cubic phases of methylammonium lead iodide. Physical Review B, 2015, 92, .	1.1	452
23	Electronic structure and stability of quaternary chalcogenide semiconductors derived from cation cross-substitution of II-VI and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>I-III-VI</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:m Physical Review B, 2009, 79, .	1.1	413
24	Can Pb-Free Halide Double Perovskites Support High-Efficiency Solar Cells?. ACS Energy Letters, 2016, 1, 949-955.	8.8	404
25	Compositional dependence of structural and electronic properties of Cu<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>ZnSn(S,Se)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow />	1.1	399
26	Synthesis, Characterization, and Electronic Structure of Single-Crystal SnS, Sn₂S₃, and SnS₂. Chemistry of Materials, 2013, 25, 4908-4916.	3.2	388
27	What Is Moving in Hybrid Halide Perovskite Solar Cells?. Accounts of Chemical Research, 2016, 49, 528-535.	7.6	385
28	Experimental and theoretical optical properties of methylammonium lead halide perovskites. Nanoscale, 2016, 8, 6317-6327.	2.8	385
29	Cation-Dependent Intrinsic Electrical Conductivity in Isostructural Tetrathiafulvalene-Based Microporous Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2015, 137, 1774-1777.	6.6	360
30	Lattice strain causes non-radiative losses in halide perovskites. Energy and Environmental Science, 2019, 12, 596-606.	15.6	343
31	Ferroelectric materials for solar energy conversion: photoferroics revisited. Energy and Environmental Science, 2015, 8, 838-848.	15.6	333
32	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
33	Real-Time Observation of Organic Cation Reorientation in Methylammonium Lead Iodide Perovskites. Journal of Physical Chemistry Letters, 2015, 6, 3663-3669.	2.1	322
34	Indirect to direct bandgap transition in methylammonium lead halide perovskite. Energy and Environmental Science, 2017, 10, 509-515.	15.6	318
35	Heterogeneous catalytic hydrogenation of CO₂by metal oxides: defect engineering â€“ perfecting imperfection. Chemical Society Reviews, 2017, 46, 4631-4644.	18.7	304
36	Metallic Conductivity in a Two-Dimensional Cobalt Dithiolene Metalâ€“Organic Framework. Journal of the American Chemical Society, 2017, 139, 10863-10867.	6.6	300

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37	Thermodynamic Origin of Photoinstability in the CH₃NH₃Pb(I_{1â€“x}Br_x)₃ Hybrid Halide Perovskite Alloy. Journal of Physical Chemistry Letters, 2016, 7, 1083-1087.	2.1	298
38	Million-Fold Electrical Conductivity Enhancement in Fe₂(DEBDC) versus Mn₂(DEBDC) (E = S, O). Journal of the American Chemical Society, 2015, 137, 6164-6167.	6.6	291
39	Interplay of Orbital and Relativistic Effects in Bismuth Oxyhalides: BiOF, BiOCl, BiOBr, and BiOI. Chemistry of Materials, 2016, 28, 1980-1984.	3.2	291
40	Principles of Chemical Bonding and Band Gap Engineering in Hybrid Organicâ€“Inorganic Halide Perovskites. Journal of Physical Chemistry C, 2015, 119, 5755-5760.	1.5	290
41	Energetic and Electronic Structure Analysis of Intrinsic Defects in SnO₂. Journal of Physical Chemistry C, 2009, 113, 439-448.	1.5	287
42	Engineering Solar Cell Absorbers by Exploring the Band Alignment and Defect Disparity: The Case of Cuâ€• and Agâ€Based Kesterite Compounds. Advanced Functional Materials, 2015, 25, 6733-6743.	7.8	284
43	Origins of band-gap renormalization in degenerately doped semiconductors. Physical Review B, 2008, 78, .	1.1	282
44	Is the Cu/Zn Disorder the Main Culprit for the Voltage Deficit in Kesterite Solar Cells?. Advanced Energy Materials, 2016, 6, 1502276.	10.2	277
45	Point defect engineering in thin-film solar cells. Nature Reviews Materials, 2018, 3, 194-210.	23.3	275
46	Enhanced Charge Transport in 2D Perovskites via Fluorination of Organic Cation. Journal of the American Chemical Society, 2019, 141, 5972-5979.	6.6	274
47	Acceptor Levels in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>p</mml:mi></mml:math>-Type<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Cu</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="bold">O</mml:mi></mml:math>: Rationalizing Theory and Experiment. Physical Review Letters, 2009, 103, 096405.	2.9	265
48	Electronic Chemical Potentials of Porous Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2014, 136, 2703-2706.	6.6	262
49	Theoretical Description of Carrier Mediated Magnetism in Cobalt Doped ZnO. Physical Review Letters, 2008, 100, 256401.	2.9	261
50	Wurtzite-derived polytypes of kesterite and stannite quaternary chalcogenide semiconductors. Physical Review B, 2010, 82, .	1.1	259
51	Conductive metalâ€“organic frameworks and networks: fact or fantasy?. Physical Chemistry Chemical Physics, 2012, 14, 13120.	1.3	258
52	Performance-limiting nanoscale trap clusters at grain junctions in halide perovskites. Nature, 2020, 580, 360-366.	13.7	255
53	Bismuth oxyhalides: synthesis, structure and photoelectrochemical activity. Chemical Science, 2016, 7, 4832-4841.	3.7	252
54	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

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55	The origin of the stereochemically active Pb(II) lone pair: DFT calculations on PbO and PbS. Journal of Solid State Chemistry, 2005, 178, 1422-1428.	1.4	243
56	Electrodeposited Aluminum-Doped Î±-Fe₂O₃ Photoelectrodes: Experiment and Theory. Chemistry of Materials, 2010, 22, 510-517.	3.2	240
57	Best practices in machine learning for chemistry. Nature Chemistry, 2021, 13, 505-508.	6.6	240
58	Band alignment of the hybrid halide perovskites CH₃NH₃PbCl₃, CH₃NH₃PbBr₃and CH₃NH₃PbI₃. Materials Horizons, 2015, 2, 228-231.	6.4	238
59	The 2019 materials by design roadmap. Journal Physics D: Applied Physics, 2019, 52, 013001.	1.3	236
60	Role of microstructure in the electronâ€“hole interaction of hybrid lead halide perovskites. Nature Photonics, 2015, 9, 695-701.	15.6	226
61	Direct Observation of Dynamic Symmetry Breaking above Room Temperature in Methylammonium Lead Iodide Perovskite. ACS Energy Letters, 2016, 1, 880-887.	8.8	221
62	Instilling defect tolerance in new compounds. Nature Materials, 2017, 16, 964-967.	13.3	219
63	An ab initio Study of Reduction of V₂O₅ through the Formation of Oxygen Vacancies and Li Intercalation. Journal of Physical Chemistry C, 2008, 112, 9903-9911.	1.5	213
64	Thermal physics of the lead chalcogenides PbS, PbSe, and PbTe from first principles. Physical Review B, 2014, 89, .	1.1	212
65	Redox-active metalâ€“organic frameworks for energy conversion and storage. Journal of Materials Chemistry A, 2019, 7, 16571-16597.	5.2	207
66	Electronic Origins of Structural Distortions in Post-Transition Metal Oxides: Experimental and Theoretical Evidence for a Revision of the Lone Pair Model. Physical Review Letters, 2006, 96, 157403.	2.9	202
67	Phase Stability of the Earth-Abundant Tin Sulfides SnS, SnS₂, and Sn₂S₃. Journal of Physical Chemistry C, 2012, 116, 24262-24267.	1.5	201
68	Electronic origins of photocatalytic activity in d0 metal organic frameworks. Scientific Reports, 2016, 6, 23676.	1.6	196
69	Giant Electronâ€“Phonon Coupling and Deep Conduction Band Resonance in Metal Halide Double Perovskite. ACS Nano, 2018, 12, 8081-8090.	7.3	190
70	The Steady Rise of Kesterite Solar Cells. ACS Energy Letters, 2017, 2, 776-779.	8.8	189
71	Revised ab initio natural band offsets of all group IV, II-VI, and III-V semiconductors. Applied Physics Letters, 2009, 94, .	1.5	188
72	Electronic structure of theÎ±andÎ´phases ofBi2O3: A combinedab initioand x-ray spectroscopy study. Physical Review B, 2006, 73, .	1.1	187

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73	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
74	Electronic structure and phase stability of MgO, ZnO, CdO, and related ternary alloys. Physical Review B, 2008, 77, .	1.1	186
75	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
76	Influence of the Anion on Lone Pair Formation in Sn(II) Monochalcogenides:â€‰ A DFT Study. Journal of Physical Chemistry B, 2005, 109, 18868-18875.	1.2	182
77	Abundance of CuZnâ€‰+â€‰SnZn and 2CuZnâ€‰+â€‰SnZn defect clusters in kesterite solar cells. Applied Physics Letters, 2012, 101, .	1.5	178
78	Research Update: Relativistic origin of slow electron-hole recombination in hybrid halide perovskite solar cells. APL Materials, 2016, 4, .	2.2	178
79	Structure, stability and work functions of the low index surfaces of pure indium oxide and Sn-doped indium oxide (ITO) from density functional theory. Journal of Materials Chemistry, 2010, 20, 10438.	6.7	177
80	Photocatalytic Carbon Dioxide Reduction with Rhodiumâ€based Catalysts in Solution and Heterogenized within Metalâ€“Organic Frameworks. ChemSusChem, 2015, 8, 603-608.	3.6	177
81	Is iron unique in promoting electrical conductivity in MOFs?. Chemical Science, 2017, 8, 4450-4457.	3.7	176
82	How Strong Is the Hydrogen Bond in Hybrid Perovskites?. Journal of Physical Chemistry Letters, 2017, 8, 6154-6159.	2.1	174
83	Dielectric and ferroic properties of metal halide perovskites. APL Materials, 2019, 7, .	2.2	173
84	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
85	Structural, magnetic, and electronic properties of the Co-Fe-Al oxide spinel system: Density-functional theory calculations. Physical Review B, 2007, 76, .	1.1	168
86	Structural diversity and electronic properties of Cu<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Sn<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

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91	Structural and electronic properties of CuSbS2 and CuBiS2: potential absorber materials for thin-film solar cells. Physical Chemistry Chemical Physics, 2012, 14, 7229.	1.3	144
92	Chemical principles underpinning the performance of the metalâ€“organic framework HKUST-1. Chemical Science, 2015, 6, 3674-3683.	3.7	144
93	Electronic Structure and Defect Physics of Tin Sulfides: SnS,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Sn</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>Sn</mml:mi><mml:mrow><mml:mi mathvariant="normal">S</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>. Physical Review Applied, 2016,	4.6	138
94	Electronic, structural, and magnetic effects of 3d transition metals in hematite. Journal of Applied Physics, 2010, 107, .	1.1	135
95	Oxidation states and ionicity. Nature Materials, 2018, 17, 958-964.	13.3	135
96	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></mml:math>. Physical Review B, 2015, 91, .	3.7	133
97	Slow Cooling of Hot Polarons in Halide Perovskite Solar Cells. ACS Energy Letters, 2017, 2, 2647-2652.	8.8	132
98	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:mrow></mml:math>NH₃PbI₃ from many-body perturbation theory. Physical Review B, 2016, 94, .	3.7	131
99	Band alignment in SnS thin-film solar cells: Possible origin of the low conversion efficiency. Applied Physics Letters, 2013, 102, .	1.5	130
100	Identification of Killer Defects in Kesterite Thin-Film Solar Cells. ACS Energy Letters, 2018, 3, 496-500.	8.8	130
101	Electronic defects in metal oxide photocatalysts. Nature Reviews Materials, 2022, 7, 503-521.	23.3	129
102	Design of I₂â€“IIâ€“IVâ€“VI₄ Semiconductors through Element Substitution: The Thermodynamic Stability Limit and Chemical Trend. Chemistry of Materials, 2014, 26, 3411-3417.	3.2	128
103	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
104	Advances in computational studies of energy materials. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2010, 368, 3379-3456.	1.6	119
105	Accumulation of Deep Traps at Grain Boundaries in Halide Perovskites. ACS Energy Letters, 2019, 4, 1321-1327.	8.8	117
106	Effect of Cr substitution on the electronic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CuAl</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>O₂. Physical Review B, 2009, 79, .	1.1	116
107	Bandgap engineering of ZnSnP2 for high-efficiency solar cells. Applied Physics Letters, 2012, 100, .	1.5	116
108	Perovskite-Inspired Photovoltaic Materials: Toward Best Practices in Materials Characterization and Calculations. Chemistry of Materials, 2017, 29, 1964-1988.	3.2	116

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109	Computational Screening of All Stoichiometric Inorganic Materials. CheM, 2016, 1, 617-627.	5.8	115
110	Stabilized tilted-octahedra halide perovskites inhibit local formation of performance-limiting phases. Science, 2021, 374, 1598-1605.	6.0	115
111	Electronic structures of rocksalt, litharge, and herzenbergite SnO by density functional theory. Physical Review B, 2004, 70, .	1.1	114
112	Electronic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>In</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub> Sn-doped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>In</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub> Physical Review B, 2010, 81, .	1.1	114
113	Polymorph Engineering of TiO₂: Demonstrating How Absolute Reference Potentials Are Determined by Local Coordination. Chemistry of Materials, 2015, 27, 3844-3851.	3.2	113
114	Perspective: Theory and simulation of hybrid halide perovskites. Journal of Chemical Physics, 2017, 146, 220901.	1.2	111
115	Assessment of polyanion (BF₄^{â^'} and PF₆^{â^'}) substitutions in hybrid halide perovskites. Journal of Materials Chemistry A, 2015, 3, 9067-9070.	5.2	108
116	Prediction of Electron Energies in Metal Oxides. Accounts of Chemical Research, 2014, 47, 364-372.	7.6	107
117	Upper limit to the photovoltaic efficiency of imperfect crystals from first principles. Energy and Environmental Science, 2020, 13, 1481-1491.	15.6	107
118	Perovskite-inspired materials for photovoltaics and beyondâ€"from design to devices. Nanotechnology, 2021, 32, 132004.	1.3	106
119	Computational materials design of crystalline solids. Chemical Society Reviews, 2016, 45, 6138-6146.	18.7	105
120	Experimental and theoretical study of the electronic structures of Î±-PbO and Î²-PbO2. Journal of Materials Chemistry, 2007, 17, 267-277.	6.7	104
121	Critical Role of Water in Defect Aggregation and Chemical Degradation of Perovskite Solar Cells. Journal of Physical Chemistry Letters, 2018, 9, 2196-2201.	2.1	104
122	Understanding the p-Type Conduction Properties of the Transparent Conducting Oxide CuBO₂: A Density Functional Theory Analysis. Chemistry of Materials, 2009, 21, 4568-4576.	3.2	100
123	Cation disorder engineering yields AgBiS2 nanocrystals with enhanced optical absorption for efficient ultrathin solar cells. Nature Photonics, 2022, 16, 235-241.	15.6	100
124	Effect of oxygen deficiency on the excited state kinetics of WO₃ and implications for photocatalysis. Chemical Science, 2019, 10, 5667-5677.	3.7	97
125	Surface Sensitivity in Lithium-Doping of MgO:â€‰ A Density Functional Theory Study with Correction for on-Site Coulomb Interactions. Journal of Physical Chemistry C, 2007, 111, 7971-7979.	1.5	96
126	Surface Energies Control the Self-Organization of Oriented In₂O₃ Nanostructures on Cubic Zirconia. Nano Letters, 2010, 10, 3740-3746.	4.5	96

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127	Influence of water intercalation and hydration on chemical decomposition and ion transport in methylammonium lead halide perovskites. Journal of Materials Chemistry A, 2018, 6, 1067-1074.	5.2	94
128	Nature of the Band Gap and Origin of the Conductivity of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>PbO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>Revealed by Theory and Experiment. Physical Review Letters, 2011, 107, 246402.	2.9	93
129	Transferable Force Field for Metalâ€“Organic Frameworks from First-Principles: BTW-FF. Journal of Chemical Theory and Computation, 2014, 10, 4644-4652.	2.3	93
130	In situ observation of picosecond polaron self-localisation in Î±-Fe2O3 photoelectrochemical cells. Nature Communications, 2019, 10, 3962.	5.8	93
131	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
132	Interplay between Order and Disorder in the High Performance of Amorphous Transparent Conducting Oxides. Chemistry of Materials, 2009, 21, 5119-5124.	3.2	90
133	The nature of electron lone pairs in BiVO4. Applied Physics Letters, 2011, 98, .	1.5	90
134	Lattice Compression Increases the Activation Barrier for Phase Segregation in Mixed-Halide Perovskites. ACS Energy Letters, 2020, 5, 3152-3158.	8.8	90
135	Influence of Rb/Cs Cation-Exchange on Inorganic Sn Halide Perovskites: From Chemical Structure to Physical Properties. Chemistry of Materials, 2017, 29, 3181-3188.	3.2	89
136	X-ray spectroscopic study of the electronic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CuCrO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml: Physical Review B, 2009, 79, .	1.1	88
137	Sustainable lead management in halide perovskite solar cells. Nature Sustainability, 2020, 3, 1044-1051.	11.5	87
138	A rapidly-reversible absorptive and emissive vapochromic Pt(II) pincer-based chemical sensor. Nature Communications, 2017, 8, 1800.	5.8	83
139	Surface oxygen vacancy origin of electron accumulation in indium oxide. Applied Physics Letters, 2011, 98, .	1.5	81
140	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
141	Electronic Structures of Antimony Oxides. Journal of Physical Chemistry C, 2013, 117, 14759-14769.	1.5	80
142	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
143	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.	3.0	79
144	Why is lead dioxide metallic?. Chemical Physics Letters, 2005, 411, 181-185.	1.2	78

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145	From kesterite to stannite photovoltaics: Stability and band gaps of the Cu2(Zn,Fe)SnS4 alloy. Applied Physics Letters, 2014, 104, .	1.5	76
146	Electronic, Energetic, and Chemical Effects of Intrinsic Defects and Fe-Doping of CoAl₂O₄: A DFT+UStudy. Journal of Physical Chemistry C, 2008, 112, 12044-12050.	1.5	75
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