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	Anharmonic lattice dynamics of superionic lithium nitride. Journal of Materials Chemistry A, 2022, 10, 2295-2304.	5.2	9
2	Pushing the boundaries of lithium battery research with atomistic modelling on different scales. Progress in Energy, 2022, 4, 012002.	4.6	12
3	From Atoms to Cells: Multiscale Modeling of LiNi_xMn_yCo_zO₂ Cathodes for Li-Ion Batteries. ACS Energy Letters, 2022, 7, 108-122.	8.8	16
4	Breaking the Aristotype: Featurization of Polyhedral Distortions in Perovskite Crystals. Chemistry of Materials, 2022, 34, 562-573.	3.2	8
5	Role of ripples in altering the electronic and chemical properties of graphene. Journal of Chemical Physics, 2022, 156, 054708.	1.2	2
6	Copper coordination polymers with selective hole conductivity. Journal of Materials Chemistry A, 2022, 10, 9582-9591.	5.2	9
7	Lone pair driven anisotropy in antimony chalcogenide semiconductors. Physical Chemistry Chemical Physics, 2022, 24, 7195-7202.	1.3	27
8	Cation disorder engineering yields AgBiS2 nanocrystals with enhanced optical absorption for efficient ultrathin solar cells. Nature Photonics, 2022, 16, 235-241.	15.6	100
9	Environmental Stability of Crystals: A Greedy Screening. Chemistry of Materials, 2022, 34, 2545-2552.	3.2	9
10	Interfacial Dipole Layer Enables High-Performance Heterojunctions for Photoelectrochemical Water Splitting. ACS Energy Letters, 2022, 7, 1392-1402.	8.8	11
11	Mixedâ€Dimensional Formamidinium Bismuth Iodides Featuring Inâ€Situ Formed Typeâ€I Band Structure for Convolution Neural Networks. Advanced Science, 2022, 9, e2200168.	5.6	8
12	Machine learned calibrations to high-throughput molecular excited state calculations. Journal of Chemical Physics, 2022, 156, 134116.	1.2	5
13	Perovskite synthesizability using graph neural networks. Npj Computational Materials, 2022, 8, .	3.5	16
14	High Power Irradiance Dependence of Charge Species Dynamics in Hybrid Perovskites and Kinetic Evidence for Transient Vibrational Stark Effect in Formamidinium. Nanomaterials, 2022, 12, 1616.	1.9	0
15	Electronic defects in metal oxide photocatalysts. Nature Reviews Materials, 2022, 7, 503-521.	23.3	129
16	Band gap opening from displacive instabilities in layered covalent-organic frameworks. Journal of Materials Chemistry A, 2022, 10, 13500-13507.	5.2	7
17	Insight into the Fergusoniteâ€“Scheelite Phase Transition of ABO₄-Type Oxides by Density Functional Theory: A Case Study of the Subtleties of the Ground State of BiVO₄. Chemistry of Materials, 2022, 34, 5334-5343.	3.2	6
18	Elucidating the origin of chiroptical activity in chiral 2D perovskites through nano-confined growth. Nature Communications, 2022, 13, .	5.8	41

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19	Switchable Electric Dipole from Polaron Localization in Dielectric Crystals. Physical Review Letters, 2022, 129, .	2.9	3
20	UnlockNN: Uncertainty quantification for neural network models of chemical systems. Journal of Open Source Software, 2022, 7, 3700.	2.0	2
21	Modeling Grain Boundaries in Polycrystalline Halide Perovskite Solar Cells. Annual Review of Condensed Matter Physics, 2021, 12, 95-109.	5.2	25
22	Multi-phonon proton transfer pathway in a molecular organic ferroelectric crystal. Physical Chemistry Chemical Physics, 2021, 23, 2885-2890.	1.3	3
23	Insights into the electric double-layer capacitance of two-dimensional electrically conductive metalâ€“organic frameworks. Journal of Materials Chemistry A, 2021, 9, 16006-16015.	5.2	31
24	Perovskite-inspired materials for photovoltaics and beyondâ€”from design to devices. Nanotechnology, 2021, 32, 132004.	1.3	106
25	Lead-free halide double perovskites: Toward stable and sustainable optoelectronic devices. Materials Today, 2021, 49, 123-144.	8.3	57
26	Passivation Properties and Formation Mechanism of Amorphous Halide Perovskite Thin Films. Advanced Functional Materials, 2021, 31, 2010330.	7.8	17
27	Solvent engineered synthesis of layered SnO for high-performance anodes. Npj 2D Materials and Applications, 2021, 5, .	3.9	11
28	Bismuth Doping Alters Structural Phase Transitions in Methylammonium Lead Tribromide Single Crystals. Journal of Physical Chemistry Letters, 2021, 12, 2749-2755.	2.1	14
29	Rapid Recombination by Cadmium Vacancies in CdTe. ACS Energy Letters, 2021, 6, 1392-1398.	8.8	39
30	Prediction of high thermoelectric performance in the low-dimensional metal halide Cs3Cu2I5. Npj Computational Materials, 2021, 7, .	3.5	26
31	Emerging inorganic solar cell efficiency tables (version 2). JPhys Energy, 2021, 3, 032003.	2.3	40
32	BiSbWO6: Properties of a mixed 5s/6s lone-pair-electron system. Chemical Physics, 2021, 544, 111117.	0.9	4
33	Correcting the corrections for charged defects in crystals. Npj Computational Materials, 2021, 7, .	3.5	17
34	Best practices in machine learning for chemistry. Nature Chemistry, 2021, 13, 505-508.	6.6	240
35	Ab initio calculation of the detailed balance limit to the photovoltaic efficiency of single p-n junction kesterite solar cells. Applied Physics Letters, 2021, 118, .	1.5	7
36	Giant Huangâ€“Rhys Factor for Electron Capture by the Iodine Intersitial in Perovskite Solar Cells. Journal of the American Chemical Society, 2021, 143, 9123-9128.	6.6	37

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37	Assessment of interstitial potentials for rapid prediction of absolute band energies in crystals. Journal of Chemical Physics, 2021, 155, 024113.	1.2	1
38	Phase Diagram and Cation Dynamics of Mixed MA_{1â€“x}FA_xPbBr₃ Hybrid Perovskites. Chemistry of Materials, 2021, 33, 5926-5934.	3.2	16
39	Low Barrier for Exciton Self-Trapping Enables High Photoluminescence Quantum Yield in Cs₃Cu₂I₅. Journal of Physical Chemistry Letters, 2021, 12, 8447-8452.	2.1	16
40	Hidden spontaneous polarisation in the chalcohalide photovoltaic absorber Sn₂SbS₂I₃. Materials Horizons, 2021, 8, 2709-2716.	6.4	24
41	Evolutionary exploration of polytypism in lead halide perovskites. Chemical Science, 2021, 12, 12165-12173.	3.7	11
42	Colloidal nano-MOFs nucleate and stabilize ultra-small quantum dots of lead bromide perovskites. Chemical Science, 2021, 12, 6129-6135.	3.7	14
43	Asymmetric carrier transport in flexible interface-type memristor enables artificial synapses with sub-femtojoule energy consumption. Nanoscale Horizons, 2021, 6, 987-997.	4.1	16
44	Enhanced visible light absorption in layered Cs₃Bi₂Br₉ through mixed-valence Sn(<scp>ii</scp>)/Sn(<scp>iv</scp>) doping. Chemical Science, 2021, 12, 14686-14699.	3.7	21
45	Self-trapping in bismuth-based semiconductors: Opportunities and challenges from optoelectronic devices to quantum technologies. Applied Physics Letters, 2021, 119, .	1.5	18
46	Atomistic models of metal halide perovskites. Matter, 2021, 4, 3867-3873.	5.0	6
47	Stabilized tilted-octahedra halide perovskites inhibit local formation of performance-limiting phases. Science, 2021, 374, 1598-1605.	6.0	115
48	Assessment of dynamic structural instabilities across 24 cubic inorganic halide perovskites. Journal of Chemical Physics, 2020, 152, 024703.	1.2	67
49	Descriptors for Electron and Hole Charge Carriers in Metal Oxides. Journal of Physical Chemistry Letters, 2020, 11, 438-444.	2.1	22
50	Bandgap lowering in mixed alloys of Cs₂Ag(Sb_xBi_{1â^'x})Br₆ double perovskite thin films. Journal of Materials Chemistry A, 2020, 8, 21780-21788.	5.2	66
51	Energy Spotlight. ACS Energy Letters, 2020, 5, 3265-3267.	8.8	0
52	Suppression of phase transitions and glass phase signatures in mixed cation halide perovskites. Nature Communications, 2020, 11, 5103.	5.8	46
53	Manganese Porphyrin Interface Engineering in Perovskite Solar Cells. ACS Applied Energy Materials, 2020, 3, 7353-7363.	2.5	17
54	Modeling the dielectric constants of crystals using machine learning. Journal of Chemical Physics, 2020, 153, 024503.	1.2	29

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55	Thermodynamic Stabilization of Mixed-Halide Perovskites against Phase Segregation. Cell Reports Physical Science, 2020, 1, 100120.	2.8	56
56	Probing the ionic defect landscape in halide perovskite solar cells. Nature Communications, 2020, 11, 6098.	5.8	75
57	Sustainable lead management in halide perovskite solar cells. Nature Sustainability, 2020, 3, 1044-1051.	11.5	87
58	Chemical Trends in the Lattice Thermal Conductivity of Li(Ni, Mn, Co)O₂ (NMC) Battery Cathodes. Chemistry of Materials, 2020, 32, 7542-7550.	3.2	28
59	Anisotropic Electron Transport Limits Performance of Bi₂WO₆ Photoanodes. Journal of Physical Chemistry C, 2020, 124, 18859-18867.	1.5	9
60	Lattice Compression Increases the Activation Barrier for Phase Segregation in Mixed-Halide Perovskites. ACS Energy Letters, 2020, 5, 3152-3158.	8.8	90
61	A density functional theory study on the interface stability between CsPbBr3 and CuI. AIP Advances, 2020, 10, .	0.6	4
62	The Holey Grail of Transparent Electronics. Matter, 2020, 3, 604-606.	5.0	2
63	Assessing the defect tolerance of kesterite-inspired solar absorbers. Energy and Environmental Science, 2020, 13, 3489-3503.	15.6	28
64	Crystal structure and metallization mechanism of the Ï€-radical metal TED. Chemical Science, 2020, 11, 11699-11704.	3.7	15
65	Hexagonal Stacking Faults Act as Hole-Blocking Layers in Lead Halide Perovskites. ACS Energy Letters, 2020, 5, 2231-2233.	8.8	12
66	Ligand engineering in Cu(<scp>ii</scp>) paddle wheel metalâ€“organic frameworks for enhanced semiconductivity. Journal of Materials Chemistry A, 2020, 8, 13160-13165.	5.2	10
67	Upper limit to the photovoltaic efficiency of imperfect crystals from first principles. Energy and Environmental Science, 2020, 13, 1481-1491.	15.6	107
68	Quick-start guide for first-principles modelling of point defects in crystalline materials. JPhys Energy, 2020, 2, 036001.	2.3	22
69	Polymorph exploration of bismuth stannate using first-principles phonon mode mapping. Chemical Science, 2020, 11, 7904-7909.	3.7	11
70	Consensus statement for stability assessment and reporting for perovskite photovoltaics based on ISOS procedures. Nature Energy, 2020, 5, 35-49.	19.8	797
71	Performance-limiting nanoscale trap clusters at grain junctions in halide perovskites. Nature, 2020, 580, 360-366.	13.7	255
72	Low-cost descriptors of electrostatic and electronic contributions to anion redox activity in batteries. IOP SciNotes, 2020, 1, 024805.	0.4	5

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73	Sn 5s2 lone pairs and the electronic structure of tin sulphides: A photoreflectance, high-energy photoemission, and theoretical investigation. Physical Review Materials, 2020, 4, .	0.9	11
74	CarrierCapture.jl: Anharmonic Carrier Capture. Journal of Open Source Software, 2020, 5, 2102.	2.0	14
75	The 2019 materials by design roadmap. Journal Physics D: Applied Physics, 2019, 52, 013001.	1.3	236
76	Role of Electronâ€“Phonon Coupling in the Thermal Evolution of Bulk Rashba-Like Spin-Split Lead Halide Perovskites Exhibiting Dual-Band Photoluminescence. ACS Energy Letters, 2019, 4, 2205-2212.	8.8	58
77	Intrinsic doping limit and defect-assisted luminescence in Cs₄PbBr₆. Journal of Materials Chemistry A, 2019, 7, 20254-20261.	5.2	48
78	Anharmonic lattice relaxation during nonradiative carrier capture. Physical Review B, 2019, 100, .	1.1	34
79	Status of materials and device modelling for kesterite solar cells. JPhys Energy, 2019, 1, 042004.	2.3	24
80	Heterostructure Engineering of a Reverse Water Gas Shift Photocatalyst. Advanced Science, 2019, 6, 1902170.	5.6	20
81	Crystal Engineering of Bi₂WO₆ to Polar Aurivillius-Phase Oxyhalides. Journal of Physical Chemistry C, 2019, 123, 29155-29161.	1.5	12
82	Data-Driven Discovery of Photoactive Quaternary Oxides Using First-Principles Machine Learning. Chemistry of Materials, 2019, 31, 7221-7230.	3.2	45
83	Highly Anisotropic Thermal Transport in LiCoO₂. Journal of Physical Chemistry Letters, 2019, 10, 5552-5556.	2.1	17
84	In situ observation of picosecond polaron self-localisation in Î±-Fe2O3 photoelectrochemical cells. Nature Communications, 2019, 10, 3962.	5.8	93
85	Charge-transfer interactions between fullerenes and a mesoporous tetrathiafulvalene-based metalâ€“organic framework. Beilstein Journal of Nanotechnology, 2019, 10, 1883-1893.	1.5	24
86	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
87	Atomistic insights into the orderâ€“disorder transition in Cu₂ZnSnS₄ solar cells from Monte Carlo simulations. Journal of Materials Chemistry A, 2019, 7, 312-321.	5.2	23
88	Lattice strain causes non-radiative losses in halide perovskites. Energy and Environmental Science, 2019, 12, 596-606.	15.6	343
89	Lone-pair effect on carrier capture in Cu₂ZnSnS₄solar cells. Journal of Materials Chemistry A, 2019, 7, 2686-2693.	5.2	55
90	Dielectric and ferroic properties of metal halide perovskites. APL Materials, 2019, 7, .	2.2	173

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91	Embrace your defects. Nature Energy, 2019, 4, 95-96.	19.8	13
92	Redox-active metalâ€“organic frameworks for energy conversion and storage. Journal of Materials Chemistry A, 2019, 7, 16571-16597.	5.2	207
93	Emerging inorganic solar cell efficiency tables (Version 1). JPhys Energy, 2019, 1, 032001.	2.3	54
94	Effect of oxygen deficiency on the excited state kinetics of WO₃ and implications for photocatalysis. Chemical Science, 2019, 10, 5667-5677.	3.7	97
95	Accumulation of Deep Traps at Grain Boundaries in Halide Perovskites. ACS Energy Letters, 2019, 4, 1321-1327.	8.8	117
96	Donor and acceptor characteristics of native point defects in GaN. Journal Physics D: Applied Physics, 2019, 52, 335104.	1.3	49
97	Vacancy-Driven Stabilization of the Cubic Perovskite Polymorph of CsPbI₃. Journal of Physical Chemistry C, 2019, 123, 9735-9744.	1.5	47
98	Enhanced Charge Transport in 2D Perovskites via Fluorination of Organic Cation. Journal of the American Chemical Society, 2019, 141, 5972-5979.	6.6	274
99	Charting a course for chemistry. Nature Chemistry, 2019, 11, 286-294.	6.6	18
100	Low-dimensional formamidinium lead perovskite architectures via controllable solvent intercalation. Journal of Materials Chemistry C, 2019, 7, 3945-3951.	2.7	23
101	Quick-start guide for first-principles modelling of semiconductor interfaces. JPhys Energy, 2019, 1, 016001.	2.3	12
102	Living in the salt-cocrystal continuum: indecisive organic complexes with thermochromic behaviour. CrystEngComm, 2019, 21, 1626-1634.	1.3	28
103	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
104	Stability and flexibility of heterometallic formate perovskites with the dimethylammonium cation: pressure-induced phase transitions. Physical Chemistry Chemical Physics, 2019, 21, 4200-4208.	1.3	10
105	Impact of nonparabolic electronic band structure on the optical and transport properties of photovoltaic materials. Physical Review B, 2019, 99, .	1.1	60
106	CO₂ Photoreduction: Heterostructure Engineering of a Reverse Water Gas Shift Photocatalyst (Adv. Sci. 22/2019). Advanced Science, 2019, 6, 1970134.	5.6	3
107	Identification of Lone-Pair Surface States on Indium Oxide. Journal of Physical Chemistry C, 2019, 123, 1700-1709.	1.5	20
108	Accelerated optimization of transparent, amorphous zinc-tin-oxide thin films for optoelectronic applications. APL Materials, 2019, 7, .	2.2	23

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109	SMACT: Semiconducting Materials by Analogy and Chemical Theory. Journal of Open Source Software, 2019, 4, 1361.	2.0	21
110	Materials discovery by chemical analogy: role of oxidation states in structure prediction. Faraday Discussions, 2018, 211, 553-568.	1.6	22
111	Intrinsic Instability of the Hybrid Halide Perovskite Semiconductor CH ₃ NH ₃ PbI ₃ [*]. Chinese Physics Letters, 2018, 35, 036104.	1.3	154
112	Vacancy defect configurations in the metalâ€“organic framework UiO-66: energetics and electronic structure. Journal of Materials Chemistry A, 2018, 6, 8507-8513.	5.2	49
113	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
114	Identification of Killer Defects in Kesterite Thin-Film Solar Cells. ACS Energy Letters, 2018, 3, 496-500.	8.8	130
115	Computer-aided design of metal chalcohalide semiconductors: from chemical composition to crystal structure. Chemical Science, 2018, 9, 1022-1030.	3.7	54
116	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
117	Water oxidation catalysed by quantum-sized BiVO₄. Journal of Materials Chemistry A, 2018, 6, 24965-24970.	5.2	10
118	Open-circuit voltage deficit in Cu2ZnSnS4 solar cells by interface bandgap narrowing. Applied Physics Letters, 2018, 113, 212103.	1.5	16
119	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
120	Oxidation states and ionicity. Nature Materials, 2018, 17, 958-964.	13.3	135
121	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
122	Stability and electronic properties of planar defects in quaternary I2-II-IV-VI4 semiconductors. Journal of Applied Physics, 2018, 124, 165705.	1.1	5
123	Preface for Special Topic: Earth abundant materials in solar cells. APL Materials, 2018, 6, .	2.2	2
124	An Unusual Phase Transition Driven by Vibrational Entropy Changes in a Hybrid Organicâ€“Inorganic Perovskite. Angewandte Chemie, 2018, 130, 9070-9074.	1.6	10
125	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
126	Prediction of multiband luminescence due to the gallium vacancyâ€“oxygen defect complex in GaN. Applied Physics Letters, 2018, 112, .	1.5	25

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127	Point defect engineering in thin-film solar cells. Nature Reviews Materials, 2018, 3, 194-210.	23.3	275
128	Giant Electronâ€“Phonon Coupling and Deep Conduction Band Resonance in Metal Halide Double Perovskite. ACS Nano, 2018, 12, 8081-8090.	7.3	190
129	Breathing-Dependent Redox Activity in a Tetrathiafulvalene-Based Metalâ€“Organic Framework. Journal of the American Chemical Society, 2018, 140, 10562-10569.	6.6	62
130	Machine learning for molecular and materials science. Nature, 2018, 559, 547-555.	13.7	2,387
131	Taking Control of Ion Transport in Halide Perovskite Solar Cells. ACS Energy Letters, 2018, 3, 1983-1990.	8.8	158
132	Role of electron-phonon coupling and thermal expansion on band gaps, carrier mobility, and interfacial offsets in kesterite thin-film solar cells. Applied Physics Letters, 2018, 112, .	1.5	19
133	Dynamic symmetry breaking and spin splitting in metal halide perovskites. Physical Review B, 2018, 98, .	1.1	52
134	Heterometallic perovskite-type metalâ€“organic framework with an ammonium cation: structure, phonons, and optical response of [NH4]Na0.5CrxAl0.5â^'x(HCOO)3 (x = 0, 0.025 and 0.5). Physical Chemistry Chemical Physics, 2018, 20, 22284-22295.	1.3	19
135	Computational Design of Photovoltaic Materials. , 2018, , 176-197.		1
136	Opposing effects of stacking faults and antisite domain boundaries on the conduction band edge in kesterite quaternary semiconductors. Physical Review Materials, 2018, 2, .	0.9	15
137	Deep vs shallow nature of oxygen vacancies and consequent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>n</mml:mi></mml:math>-type carrier concentrations in transparent conducting oxides. Physical Review Materials, 2018, 2, .	0.9	73
138	Perovskite-Inspired Photovoltaic Materials: Toward Best Practices in Materials Characterization and Calculations. Chemistry of Materials, 2017, 29, 1964-1988.	3.2	116
139	Self-Consistent Hybrid Functional Calculations: Implications for Structural, Electronic, and Optical Properties of Oxide Semiconductors. Nanoscale Research Letters, 2017, 12, 19.	3.1	34
140	The Steady Rise of Kesterite Solar Cells. ACS Energy Letters, 2017, 2, 776-779.	8.8	189
141	The Organic Secondary Building Unit: Strong Intermolecular Ï€ Interactions Define Topology in MIT-25, a Mesoporous MOF with Proton-Replete Channels. Journal of the American Chemical Society, 2017, 139, 3619-3622.	6.6	72
142	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
143	Chemical and Lattice Stability of the Tin Sulfides. Journal of Physical Chemistry C, 2017, 121, 6446-6454.	1.5	73
144	Is iron unique in promoting electrical conductivity in MOFs?. Chemical Science, 2017, 8, 4450-4457.	3.7	176

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145	DFT investigation into the underperformance of sulfide materials in photovoltaic applications. Journal of Materials Chemistry A, 2017, 5, 9132-9140.	5.2	19
146	Trimethylsulfonium Lead Triiodide: An Air-Stable Hybrid Halide Perovskite. Inorganic Chemistry, 2017, 56, 6302-6309.	1.9	52
147	Electron Counting in Solids: Oxidation States, Partial Charges, and Ionicity. Journal of Physical Chemistry Letters, 2017, 8, 2074-2075.	2.1	65
148	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
149	Vacuum-annealing induces sub-surface redox-states in surfactant-structured Î±-Fe2O3 photoanodes prepared by ink-jet printing. Applied Catalysis B: Environmental, 2017, 211, 289-295.	10.8	14
150	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.	0.8	16
151	Designing porous electronic thin-film devices: band offsets and heteroepitaxy. Faraday Discussions, 2017, 201, 207-219.	1.6	36
152	Heterogeneous catalytic hydrogenation of CO₂by metal oxides: defect engineering â€“ perfecting imperfection. Chemical Society Reviews, 2017, 46, 4631-4644.	18.7	304
153	Perspective: Theory and simulation of hybrid halide perovskites. Journal of Chemical Physics, 2017, 146, 220901.	1.2	111
154	Electroactive Nanoporous Metal Oxides and Chalcogenides by Chemical Design. Chemistry of Materials, 2017, 29, 3663-3670.	3.2	8
155	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
156	Metastable cubic tin sulfide: A novel phonon-stable chiral semiconductor. APL Materials, 2017, 5, 036101.	2.2	51
157	Theory of ionization potentials of nonmetallic solids. Physical Review B, 2017, 95, .	1.1	18
158	Indirect to direct bandgap transition in methylammonium lead halide perovskite. Energy and Environmental Science, 2017, 10, 509-515.	15.6	318
159	Quantifying Thermal Disorder in Metalâ€“Organic Frameworks: Lattice Dynamics and Molecular Dynamics Simulations of Hybrid Formate Perovskites. Journal of Physical Chemistry C, 2017, 121, 421-429.	1.5	16
160	H-Center and V-Center Defects in Hybrid Halide Perovskites. ACS Energy Letters, 2017, 2, 2713-2714.	8.8	47
161	Revisiting the Incorporation of Ti(IV) in UiO-type Metalâ€“Organic Frameworks: Metal Exchange versus Grafting and Their Implications on Photocatalysis. Chemistry of Materials, 2017, 29, 8963-8967.	3.2	64
162	Slow Cooling of Hot Polarons in Halide Perovskite Solar Cells. ACS Energy Letters, 2017, 2, 2647-2652.	8.8	132

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163	MOFs modeling and theory: general discussion. Faraday Discussions, 2017, 201, 233-245.	1.6	4
164	Electronic, magnetic and photophysical properties of MOFs and COFs: general discussion. Faraday Discussions, 2017, 201, 87-99.	1.6	9
165	New directions in gas sorption and separation with MOFs: general discussion. Faraday Discussions, 2017, 201, 175-194.	1.6	6
166	Catalysis in MOFs: general discussion. Faraday Discussions, 2017, 201, 369-394.	1.6	14
167	Anharmonic Origin of Giant Thermal Displacements in the Metalâ€“Organic Framework UiO-67. Journal of Physical Chemistry C, 2017, 121, 22010-22014.	1.5	3
168	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
169	Temperature-Induced Large Broadening and Blue Shift in the Electronic Band Structure and Optical Absorption of Methylammonium Lead Iodide Perovskite. Journal of Physical Chemistry Letters, 2017, 8, 3720-3725.	2.1	29
170	Electronic structure design for nanoporous, electrically conductive zeolitic imidazolate frameworks. Journal of Materials Chemistry C, 2017, 5, 7726-7731.	2.7	40
171	Candidate photoferroic absorber materials for thin-film solar cells from naturally occurring minerals: enargite, stephanite, and bournonite. Sustainable Energy and Fuels, 2017, 1, 1339-1350.	2.5	32
172	How Strong Is the Hydrogen Bond in Hybrid Perovskites?. Journal of Physical Chemistry Letters, 2017, 8, 6154-6159.	2.1	174
173	A rapidly-reversible absorptive and emissive vapochromic Pt(II) pincer-based chemical sensor. Nature Communications, 2017, 8, 1800.	5.8	83
174	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
175	Low-frequency optical phonon modes and carrier mobility in the halide perovskite CH3NH3PbBr3 using terahertz time-domain spectroscopy. Applied Physics Letters, 2017, 111, .	1.5	54
176	Metallic Conductivity in a Two-Dimensional Cobalt Dithiolene Metalâ€“Organic Framework. Journal of the American Chemical Society, 2017, 139, 10863-10867.	6.6	300
177	Ab initio lattice dynamics for materials design and characterisation. Acta Crystallographica Section A: Foundations and Advances, 2017, 73, C77-C77.	0.0	0
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