Aron Walsh

List of Publications by Citations

401 papers	42,272 citations	99 h-index	198 g-index
483 ext. papers	48,909 ext. citations	9.4 avg, IF	8.04 L-index

#	Paper	IF	Citations
401	Nanocrystals of Cesium Lead Halide Perovskites (CsPbX□X = Cl, Br, and I): Novel Optoelectronic Materials Showing Bright Emission with Wide Color Gamut. *Nano Letters*, **2015**, 15, 3692-6	11.5	4888
400	Atomistic origins of high-performance in hybrid halide perovskite solar cells. *Nano Letters*, **2014**, 14, 2584-90	11.5	1756
399	Band alignment of rutile and anatase TiO□*Nature Materials*, **2013**, 12, 798-801	27	1656
398	Ionic transport in hybrid lead iodide perovskite solar cells. *Nature Communications*, **2015**, 6, 7497	17.4	1649
397	Machine learning for molecular and materials science. *Nature*, **2018**, 559, 547-555	50.4	1282
396	Classification of lattice defects in the kesterite Cu2ZnSnS4 and Cu2ZnSnSe4 earth-abundant solar cell absorbers. *Advanced Materials*, **2013**, 25, 1522-39	24	979
395	Band Edge Electronic Structure of BiVO4: Elucidating the Role of the Bi s and V d Orbitals. *Chemistry of Materials*, **2009**, 21, 547-551	9.6	542
394	Engineering the optical response of the titanium-MIL-125 metal-organic framework through ligand functionalization. *Journal of the American Chemical Society*, **2013**, 135, 10942-5	16.4	535
393	Intrinsic point defects and complexes in the quaternary kesterite semiconductor Cu2ZnSnS4. *Physical Review B*, **2010**, 81,	3.3	532
392	Crystal and electronic band structure of Cu2ZnSnX4 (X=S and Se) photovoltaic absorbers: First-principles insights. *Applied Physics Letters*, **2009**, 94, 041903	3.4	526
391	Relativistic quasiparticle self-consistent electronic structure of hybrid halide perovskite photovoltaic absorbers. *Physical Review B*, **2014**, 89,	3.3	514
390	Nature of the band gap of In2O3 revealed by first-principles calculations and x-ray spectroscopy. *Physical Review Letters*, **2008**, 100, 167402	7.4	498
389	Kesterite Thin-Film Solar Cells: Advances in Materials Modelling of Cu2ZnSnS4. *Advanced Energy Materials*, **2012**, 2, 400-409	21.8	488
388	Structural and electronic properties of hybrid perovskites for high-efficiency thin-film photovoltaics from first-principles. *APL Materials*, **2013**, 1, 042111	5.7	462
387	Stereochemistry of post-transition metal oxides: revision of the classical lone pair model. *Chemical Society Reviews*, **2011**, 40, 4455-63	58.5	456
386	The dynamics of methylammonium ions in hybrid organic-inorganic perovskite solar cells. *Nature Communications*, **2015**, 6, 7124	17.4	446
385	Molecular ferroelectric contributions to anomalous hysteresis in hybrid perovskite solar cells. *APL Materials*, **2014**, 2, 081506	5.7	443

384	Defect physics of the kesterite thin-film solar cell absorber Cu2ZnSnS4. *Applied Physics Letters*, **2010**, 96, 021902	3.4	405
383	Self-regulation mechanism for charged point defects in hybrid halide perovskites. *Angewandte Chemie - International Edition*, **2015**, 54, 1791-4	16.4	394
382	Consensus statement for stability assessment and reporting for perovskite photovoltaics based on ISOS procedures. *Nature Energy*, **2020**, 5, 35-49	62.3	369
381	Lattice dynamics and vibrational spectra of the orthorhombic, tetragonal, and cubic phases of methylammonium lead iodide. *Physical Review B*, **2015**, 92,	3.3	360
380	Electronic structure and stability of quaternary chalcogenide semiconductors derived from cation cross-substitution of II-VI and I-III-VI2 compounds. *Physical Review B*, **2009**, 79,	3.3	359
379	Compositional dependence of structural and electronic properties of Cu2ZnSn(S,Se)4 alloys for thin film solar cells. *Physical Review B*, **2011**, 83,	3.3	350
378	Cubic Perovskite Structure of Black Formamidinium Lead Iodide, [HC(NH2)2]PbI3, at 298 K. *Journal of Physical Chemistry Letters*, **2015**, 6, 3209-3212	6.4	343
377	Synthesis, Characterization, and Electronic Structure of Single-Crystal SnS, Sn2S3, and SnS2. *Chemistry of Materials*, **2013**, 25, 4908-4916	9.6	321
376	What Is Moving in Hybrid Halide Perovskite Solar Cells?. *Accounts of Chemical Research*, **2016**, 49, 528-35	24.3	319
375	Can Pb-Free Halide Double Perovskites Support High-Efficiency Solar Cells?. *ACS Energy Letters*, **2016**, 1, 949-955	20.1	301
374	Experimental and theoretical optical properties of methylammonium lead halide perovskites. *Nanoscale*, **2016**, 8, 6317-27	7.7	287
373	Cation-dependent intrinsic electrical conductivity in isostructural tetrathiafulvalene-based microporous metal-organic frameworks. *Journal of the American Chemical Society*, **2015**, 137, 1774-7	16.4	282
372	Real-Time Observation of Organic Cation Reorientation in Methylammonium Lead Iodide Perovskites. *Journal of Physical Chemistry Letters*, **2015**, 6, 3663-9	6.4	281
371	Ferroelectric materials for solar energy conversion: photoferroics revisited. *Energy and Environmental Science*, **2015**, 8, 838-848	35.4	260
370	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	3.6	243
369	Theoretical description of carrier mediated magnetism in cobalt doped ZnO. *Physical Review Letters* , **2008**, 100, 256401	7.4	240
368	Indirect to direct bandgap transition in methylammonium lead halide perovskite. *Energy and Environmental Science*, **2017**, 10, 509-515	35.4	237
367	Acceptor levels in p-type Cu(2)O: rationalizing theory and experiment. *Physical Review Letters*, **2009** , 103, 096405	7.4	237

366	Energetic and Electronic Structure Analysis of Intrinsic Defects in SnO2. *Journal of Physical Chemistry C*, **2009**, 113, 439-448	3.8	236
365	Origins of band-gap renormalization in degenerately doped semiconductors. *Physical Review B*, **2008**, 78,	3.3	235
364	Principles of Chemical Bonding and Band Gap Engineering in Hybrid Organic-Inorganic Halide Perovskites. *Journal of Physical Chemistry C*, **2015**, 119, 5755-5760	3.8	226
363	Interplay of Orbital and Relativistic Effects in Bismuth Oxyhalides: BiOF, BiOCl, BiOBr, and BiOI. *Chemistry of Materials*, **2016**, 28, 1980-1984	9.6	225
362	Million-Fold Electrical Conductivity Enhancement in Fe2(DEBDC) versus Mn2(DEBDC) (E = S, O). *Journal of the American Chemical Society*, **2015**, 137, 6164-7	16.4	222
361	Conductive metal-organic frameworks and networks: fact or fantasy?. *Physical Chemistry Chemical Physics*, **2012**, 14, 13120-32	3.6	222
360	Electronic chemical potentials of porous metal-organic frameworks. *Journal of the American Chemical Society*, **2014**, 136, 2703-6	16.4	221
359	Is the Cu/Zn Disorder the Main Culprit for the Voltage Deficit in Kesterite Solar Cells?. *Advanced Energy Materials*, **2016**, 6, 1502276	21.8	221
358	Wurtzite-derived polytypes of kesterite and stannite quaternary chalcogenide semiconductors. *Physical Review B*, **2010**, 82,	3.3	220
357	Engineering Solar Cell Absorbers by Exploring the Band Alignment and Defect Disparity: The Case of Cu- and Ag-Based Kesterite Compounds. *Advanced Functional Materials*, **2015**, 25, 6733-6743	15.6	218
356	Thermodynamic Origin of Photoinstability in the CH3NH3Pb(I1-xBrx)3 Hybrid Halide Perovskite Alloy. *Journal of Physical Chemistry Letters*, **2016**, 7, 1083-7	6.4	217
355	Heterogeneous catalytic hydrogenation of CO by metal oxides: defect engineering - perfecting imperfection. *Chemical Society Reviews*, **2017**, 46, 4631-4644	58.5	212
354	Lattice strain causes non-radiative losses in halide perovskites. *Energy and Environmental Science*, **2019**, 12, 596-606	35.4	211
353	Metallic Conductivity in a Two-Dimensional Cobalt Dithiolene Metal-Organic Framework. *Journal of the American Chemical Society*, **2017**, 139, 10863-10867	16.4	209
352	Electrodeposited Aluminum-Doped □Fe2O3 Photoelectrodes: Experiment and Theory. *Chemistry of Materials*, **2010**, 22, 510-517	9.6	207
351	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	3.3	207
350	Role of Microstructure in the Electron-Hole Interaction of Hybrid Lead-Halide Perovskites. *Nature Photonics*, **2015**, 9, 695-701	33.9	203
349	Band alignment of the hybrid halide perovskites CH3NH3PbCl3, CH3NH3PbBr3 and CH3NH3PbI3. *Materials Horizons*, **2015**, 2, 228-231	14.4	198

348	Bismuth oxyhalides: synthesis, structure and photoelectrochemical activity. *Chemical Science*, **2016**, 7, 4832-4841	9.4	197
347	Electronic and optical properties of single crystal SnS2: an earth-abundant disulfide photocatalyst. *Journal of Materials Chemistry A*, **2016**, 4, 1312-1318	13	190
346	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	7.4	182
345	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	3.8	181
344	Direct Observation of Dynamic Symmetry Breaking above Room Temperature in Methylammonium Lead Iodide Perovskite. *ACS Energy Letters*, **2016**, 1, 880-887	20.1	177
343	Point defect engineering in thin-film solar cells. *Nature Reviews Materials*, **2018**, 3, 194-210	73.3	176
342	Thermal physics of the lead chalcogenides PbS, PbSe, and PbTe from first principles. *Physical Review B*, **2014**, 89,	3.3	172
341	Phase Stability of the Earth-Abundant Tin Sulfides SnS, SnS2, and Sn2S3. *Journal of Physical Chemistry C*, **2012**, 116, 24262-24267	3.8	172
340	Enhanced Charge Transport in 2D Perovskites via Fluorination of Organic Cation. *Journal of the American Chemical Society*, **2019**, 141, 5972-5979	16.4	170
339	Electronic structure of the □and □phases of Bi2O3: A combined ab initio and x-ray spectroscopy study. *Physical Review B*, **2006**, 73,	3.3	168
338	Electronic structure and phase stability of MgO, ZnO, CdO, and related ternary alloys. *Physical Review B*, **2008**, 77,	3.3	167
337	Revised ab initio natural band offsets of all group IV, II-VI, and III-V semiconductors. *Applied Physics Letters*, **2009**, 94, 212109	3.4	162
336	Predicting synthesizability. *Journal Physics D: Applied Physics*, **2019**, 52,	3	161
335	Instilling defect tolerance in new compounds. *Nature Materials*, **2017**,	27	156
334	Performance-limiting nanoscale trap clusters at grain junctions in halide perovskites. *Nature*, **2020**, 580, 360-366	50.4	155
333	Electronic origins of photocatalytic activity in d0 metal organic frameworks. *Scientific Reports*, **2016**, 6, 23676	4.9	154
332	Research Update: Relativistic origin of slow electron-hole recombination in hybrid halide perovskite solar cells. *APL Materials*, **2016**, 4, 091501	5.7	153
331	Structural diversity and electronic properties of Cu2SnX3 (X=S, Se): A first-principles investigation. *Physical Review B*, **2011**, 84,	3.3	152

330	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		150
329	Photocatalytic carbon dioxide reduction with rhodium-based catalysts in solution and heterogenized within metal-organic frameworks. *ChemSusChem*, **2015**, 8, 603-8	8.3	149
328	Influence of the anion on lone pair formation in Sn(II) monochalcogenides: a DFT study. *Journal of Physical Chemistry B*, **2005**, 109, 18868-75	3.4	149
327	Insights into the structure of the stable and metastable (GeTe)m(Sb2Te3)n compounds. *Physical Review B*, **2008**, 78,	3.3	147
326	The Steady Rise of Kesterite Solar Cells. *ACS Energy Letters*, **2017**, 2, 776-779	20.1	144
325	Abundance of CuZn + SnZn and 2CuZn + SnZn defect clusters in kesterite solar cells. *Applied Physics Letters*, **2012**, 101, 223901	3.4	140
324	Structural, magnetic, and electronic properties of the Co-Fe-Al oxide spinel system: Density-functional theory calculations. *Physical Review B*, **2007**, 76,	3.3	134
323	Redox-active metal–organic frameworks for energy conversion and storage. *Journal of Materials Chemistry A*, **2019**, 7, 16571-16597	13	127
322	Spontaneous Octahedral Tilting in the Cubic Inorganic Cesium Halide Perovskites CsSnX and CsPbX (X = F, Cl, Br, I). *Journal of Physical Chemistry Letters*, **2017**, 8, 4720-4726	6.4	126
321	Giant Electron-Phonon Coupling and Deep Conduction Band Resonance in Metal Halide Double Perovskite. *ACS Nano*, **2018**, 12, 8081-8090	16.7	123
320	Structural and electronic properties of CuSbS2 and CuBiS2: potential absorber materials for thin-film solar cells. *Physical Chemistry Chemical Physics*, **2012**, 14, 7229-33	3.6	123
319	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	9.6	123
318	Taking Control of Ion Transport in Halide Perovskite Solar Cells. *ACS Energy Letters*, **2018**, 3, 1983-1990	20.1	121
317	Band alignment in SnS thin-film solar cells: Possible origin of the low conversion efficiency. *Applied Physics Letters*, **2013**, 102, 132111	3.4	119
316	Electronic Structure and Defect Physics of Tin Sulfides: SnS, Sn2S3, and SnS2. *Physical Review Applied*, **2016**, 6,	4.3	111
315	Electronic, structural, and magnetic effects of 3d transition metals in hematite. *Journal of Applied Physics*, **2010**, 107, 123712	2.5	111
314	How Strong Is the Hydrogen Bond in Hybrid Perovskites?. *Journal of Physical Chemistry Letters*, **2017**, 8, 6154-6159	6.4	110
313	Advances in computational studies of energy materials. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2010**, 368, 3379-456	3	110

312	Design of I2□IVV□I4 Semiconductors through Element Substitution: The Thermodynamic Stability Limit and Chemical Trend. *Chemistry of Materials*, **2014**, 26, 3411-3417	9.6	109
311	Lattice dynamics of the tin sulphides SnS, SnS and SnS: vibrational spectra and thermal transport. *Physical Chemistry Chemical Physics*, **2017**, 19, 12452-12465	3.6	108
310	Dielectric and ferroic properties of metal halide perovskites. *APL Materials*, **2019**, 7, 010901	5.7	108
309	Intrinsic Instability of the Hybrid Halide Perovskite Semiconductor CH 3 NH 3 PbI 3 *. *Chinese Physics Letters*, **2018**, 35, 036104	1.8	107
308	Is iron unique in promoting electrical conductivity in MOFs?. *Chemical Science*, **2017**, 8, 4450-4457	9.4	106
307	Electronic structures of rocksalt, litharge, and herzenbergite SnO by density functional theory. *Physical Review B*, **2004**, 70,	3.3	105
306	Anharmonicity in the High-Temperature Cmcm Phase of SnSe: Soft Modes and Three-Phonon Interactions. *Physical Review Letters*, **2016**, 117, 075502	7.4	104
305	Effect of Cr substitution on the electronic structure of CuAl1⊠CrxO2. *Physical Review B*, **2009**, 79,	3.3	102
304	Phase stability and transformations in the halide perovskite CsSnI3. *Physical Review B*, **2015**, 91,	3.3	101
303	Phonon anharmonicity, lifetimes, and thermal transport in CH3NH3PbI3 from many-body perturbation theory. *Physical Review B*, **2016**, 94,	3.3	101
302	Bandgap engineering of ZnSnP2 for high-efficiency solar cells. *Applied Physics Letters*, **2012**, 100, 251911	3.4	99
301	Relativistic electronic structure and band alignment of BiSI and BiSeI: candidate photovoltaic materials. *Journal of Materials Chemistry A*, **2016**, 4, 2060-2068	13	97
300	Chemical principles underpinning the performance of the metal-organic framework HKUST-1. *Chemical Science*, **2015**, 6, 3674-3683	9.4	96
299	Slow Cooling of Hot Polarons in Halide Perovskite Solar Cells. *ACS Energy Letters*, **2017**, 2, 2647-2652	20.1	94
298	Prediction of electron energies in metal oxides. *Accounts of Chemical Research*, **2014**, 47, 364-72	24.3	94
297	Electronic structure of In2O3 and Sn-doped In2O3 by hard x-ray photoemission spectroscopy. *Physical Review B*, **2010**, 81,	3.3	94
296	Polymorph Engineering of TiO2: Demonstrating How Absolute Reference Potentials Are Determined by Local Coordination. *Chemistry of Materials*, **2015**, 27, 3844-3851	9.6	92
295	Experimental and theoretical study of the electronic structures of □PbO and □PbO2. *Journal of Materials Chemistry*, **2007**, 17, 267-277		92

294	Surface Sensitivity in Lithium-Doping of MgO: A Density Functional Theory Study with Correction for on-Site Coulomb Interactions. *Journal of Physical Chemistry C*, **2007**, 111, 7971-7979	3.8	91
293	Oxidation states and ionicity. *Nature Materials*, **2018**, 17, 958-964	27	91
292	Surface energies control the self-organization of oriented In2O3 nanostructures on cubic zirconia. *Nano Letters*, **2010**, 10, 3740-6	11.5	90
291	Understanding the p-Type Conduction Properties of the Transparent Conducting Oxide CuBO2: A Density Functional Theory Analysis. *Chemistry of Materials*, **2009**, 21, 4568-4576	9.6	89
290	Identification of Killer Defects in Kesterite Thin-Film Solar Cells. *ACS Energy Letters*, **2018**, 3, 496-500	20.1	88
289	Perovskite-Inspired Photovoltaic Materials: Toward Best Practices in Materials Characterization and Calculations. *Chemistry of Materials*, **2017**, 29, 1964-1988	9.6	87
288	Perspective: Theory and simulation of hybrid halide perovskites. *Journal of Chemical Physics*, **2017**, 146, 220901	3.9	87
287	Self-Regulation Mechanism for Charged Point Defects in Hybrid Halide Perovskites. *Angewandte Chemie*, **2015**, 127, 1811-1814	3.6	87
286	Assessment of polyanion (BF4 and PF6) substitutions in hybrid halide perovskites. *Journal of Materials Chemistry A*, **2015**, 3, 9067-9070	13	83
285	X-ray spectroscopic study of the electronic structure of CuCrO2. *Physical Review B*, **2009**, 79,	3.3	82
284	The nature of electron lone pairs in BiVO4. *Applied Physics Letters*, **2011**, 98, 212110	3.4	81
283	Interplay between Order and Disorder in the High Performance of Amorphous Transparent Conducting Oxides. *Chemistry of Materials*, **2009**, 21, 5119-5124	9.6	80
282	Accumulation of Deep Traps at Grain Boundaries in Halide Perovskites. *ACS Energy Letters*, **2019**, 4, 1321-1327	20.1	76
281	Nature of the band gap and origin of the conductivity of PbO2 revealed by theory and experiment. *Physical Review Letters*, **2011**, 107, 246402	7.4	76
280	Surface oxygen vacancy origin of electron accumulation in indium oxide. *Applied Physics Letters*, **2011**, 98, 261910	3.4	75
279	Origin of electronic and optical trends in ternary In2O3(ZnO)n transparent conducting oxides (n=1,3,5): Hybrid density functional theory calculations. *Physical Review B*, **2009**, 79,	3.3	73
278	Critical Role of Water in Defect Aggregation and Chemical Degradation of Perovskite Solar Cells. *Journal of Physical Chemistry Letters*, **2018**, 9, 2196-2201	6.4	72
277	Computational Screening of All Stoichiometric Inorganic Materials. *CheM*, **2016**, 1, 617-627	16.2	72

276	Computational materials design of crystalline solids. *Chemical Society Reviews*, **2016**, 45, 6138-6146	58.5	72
275	Transferable Force Field for Metal-Organic Frameworks from First-Principles: BTW-FF. *Journal of Chemical Theory and Computation*, **2014**, 10, 4644-4652	6.4	69
274	Electronic structure modulation of metal-organic frameworks for hybrid devices. *ACS Applied Materials & Interfaces*, **2014**, 6, 22044-50	9.5	67
273	Electronic, Energetic, and Chemical Effects of Intrinsic Defects and Fe-Doping of CoAl2O4: A DFT+U Study. *Journal of Physical Chemistry C*, **2008**, 112, 12044-12050	3.8	66
272	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	13	64
271	Electronic Structures of Antimony Oxides. *Journal of Physical Chemistry C*, **2013**, 117, 14759-14769	3.8	62
270	Influence of Rb/Cs Cation-Exchange on Inorganic Sn Halide Perovskites: From Chemical Structure to Physical Properties. *Chemistry of Materials*, **2017**, 29, 3181-3188	9.6	61
269	Origin of deep subgap states in amorphous indium gallium zinc oxide: Chemically disordered coordination of oxygen. *Applied Physics Letters*, **2014**, 104, 232108	3.4	61
268	Best practices in machine learning for chemistry. *Nature Chemistry*, **2021**, 13, 505-508	17.6	61
267	Influence of the exchange-correlation functional on the quasi-harmonic lattice dynamics of II-VI semiconductors. *Journal of Chemical Physics*, **2015**, 143, 064710	3.9	60
266	Group-IIIA versus IIIB delafossites: Electronic structure study. *Physical Review B*, **2009**, 80,	3.3	60
265	Strontium migration assisted by oxygen vacancies in SrTiO3 from classical and quantum mechanical simulations. *Physical Review B*, **2011**, 83,	3.3	60
264	The Organic Secondary Building Unit: Strong Intermolecular Interactions Define Topology in MIT-25, a Mesoporous MOF with Proton-Replete Channels. *Journal of the American Chemical Society* , **2017**, 139, 3619-3622	16.4	59
263	Role of entropic effects in controlling the polymorphism in formate ABX3 metal-organic frameworks. *Chemical Communications*, **2015**, 51, 15538-41	5.8	59
262	From kesterite to stannite photovoltaics: Stability and band gaps of the Cu2(Zn,Fe)SnS4 alloy. *Applied Physics Letters*, **2014**, 104, 021912	3.4	59
261	Physical Properties, Intrinsic Defects, and Phase Stability of Indium Sesquioxide. *Chemistry of Materials*, **2009**, 21, 4962-4969	9.6	59
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259	Upper limit to the photovoltaic efficiency of imperfect crystals from first principles. *Energy and Environmental Science*, **2020**, 13, 1481-1491	35.4	58

258	Electron excess in alkaline earth sub-nitrides: 2D electron gas or 3D electride?. *Journal of Materials Chemistry C*, **2013**, 1, 3525	7.1	58
257	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
256	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
255	Effect of oxygen deficiency on the excited state kinetics of WO and implications for photocatalysis. *Chemical Science*, **2019**, 10, 5667-5677	9.4	56
254	A rapidly-reversible absorptive and emissive vapochromic Pt(II) pincer-based chemical sensor. *Nature Communications*, **2017**, 8, 1800	17.4	56
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252	Ternary cobalt spinel oxides for solar driven hydrogen production: Theory and experiment. *Energy and Environmental Science*, **2009**, 2, 774	35.4	55
251	Helical frontier orbitals of conjugated linear molecules. *Chemical Science*, **2013**, 4, 4278	9.4	53
250	Ellipsometric characterization and density-functional theory analysis of anisotropic optical properties of single-crystal □SnS. *Journal of Applied Physics*, **2014**, 116, 013511	2.5	53
249	Chemical and Lattice Stability of the Tin Sulfides. *Journal of Physical Chemistry C*, **2017**, 121, 6446-6454	3.8	52
248	Revisiting the Incorporation of Ti(IV) in UiO-type Metal□Organic Frameworks: Metal Exchange versus Grafting and Their Implications on Photocatalysis. *Chemistry of Materials*, **2017**, 29, 8963-8967	9.6	52
247	In situ observation of picosecond polaron self-localisation in □FeO photoelectrochemical cells. *Nature Communications*, **2019**, 10, 3962	17.4	52
246	Role of Amine□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	9.6	52
245	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	11.5	52
244	Modular design of SPIRO-OMeTAD analogues as hole transport materials in solar cells. *Chemical Communications*, **2015**, 51, 8935-8	5.8	51
243	Band structure engineering of multinary chalcogenide topological insulators. *Physical Review B*, **2011**, 83,	3.3	51
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241	Microscopic origins of electron and hole stability in ZnO. *Chemical Communications*, **2011**, 47, 3386-8	5.8	50

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238	Organised chaos: entropy in hybrid inorganic-organic systems and other materials. *Chemical Science* , **2016**, 7, 6316-6324	9.4	49
237	Breathing-Dependent Redox Activity in a Tetrathiafulvalene-Based Metal-Organic Framework. *Journal of the American Chemical Society*, **2018**, 140, 10562-10569	16.4	48
236	Experimental and theoretical study of the electronic structure of HgO and Tl2O3. *Physical Review B*, **2005**, 71,	3.3	48
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234	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
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230	Ligand design for long-range magnetic order in metal-organic frameworks. *Chemical Communications*, **2014**, 50, 13990-3	5.8	44
229	Catalytic Amine Oxidation under Ambient Aerobic Conditions: Mimicry of Monoamine Oxidase B. *Angewandte Chemie - International Edition*, **2015**, 54, 8997-9000	16.4	43
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