Aron Walsh

List of Publications by Year in Descending Order

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	Breaking the Aristotype: Featurization of Polyhedral Distortions in Perovskite Crystals. *Chemistry of Materials*, **2022**, 34, 562-573	9.6	1
400	Role of ripples in altering the electronic and chemical properties of graphene.. *Journal of Chemical Physics*, **2022**, 156, 054708	3.9	1
399	Lone pair driven anisotropy in antimony chalcogenide semiconductors.. *Physical Chemistry Chemical Physics*, **2022**,	3.6	3
398	Cation disorder engineering yields AgBiS2 nanocrystals with enhanced optical absorption for efficient ultrathin solar cells. *Nature Photonics*, **2022**, 16, 235-241	33.9	19
397	Environmental Stability of Crystals: A Greedy Screening.. *Chemistry of Materials*, **2022**, 34, 2545-2552	9.6	0
396	Interfacial Dipole Layer Enables High-Performance Heterojunctions for Photoelectrochemical Water Splitting. *ACS Energy Letters*, **2022**, 7, 1392-1402	20.1	2
395	Mixed-Dimensional Formamidinium Bismuth Iodides Featuring In-Situ Formed Type-I Band Structure for Convolution Neural Networks.. *Advanced Science*, **2022**, e2200168	13.6	2
394	Machine learned calibrations to high-throughput molecular excited state calculations.. *Journal of Chemical Physics*, **2022**, 156, 134116	3.9	2
393	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	5.4	
392	Self-trapping in bismuth-based semiconductors: Opportunities and challenges from optoelectronic devices to quantum technologies. *Applied Physics Letters*, **2021**, 119, 220501	3.4	1
391	Atomistic models of metal halide perovskites. *Matter*, **2021**, 4, 3867-3873	12.7	2
390	Asymmetric carrier transport in flexible interface-type memristor enables artificial synapses with sub-femtojoule energy consumption. *Nanoscale Horizons*, **2021**, 6, 987-997	10.8	5
389	Enhanced visible light absorption in layered CsBiBr through mixed-valence Sn(ii)/Sn(iv) doping. *Chemical Science*, **2021**, 12, 14686-14699	9.4	8
388	Bismuth Doping Alters Structural Phase Transitions in Methylammonium Lead Tribromide Single Crystals. *Journal of Physical Chemistry Letters*, **2021**, 12, 2749-2755	6.4	6
387	Rapid Recombination by Cadmium Vacancies in CdTe. *ACS Energy Letters*, **2021**, 6, 1392-1398	20.1	12
386	Prediction of high thermoelectric performance in the low-dimensional metal halide Cs3Cu2I5. *Npj Computational Materials*, **2021**, 7,	10.9	7
385	Emerging inorganic solar cell efficiency tables (version 2). *JPhys Energy*, **2021**, 3, 032003	4.9	15

384	BiSbWO6: Properties of a mixed 5s/6s lone-pair-electron system. *Chemical Physics*, **2021**, 544, 111117	2.3	0
383	Best practices in machine learning for chemistry. *Nature Chemistry*, **2021**, 13, 505-508	17.6	61
382	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, 243905	3.4	1
381	Giant Huang-Rhys Factor for Electron Capture by the Iodine Intersitial in Perovskite Solar Cells. *Journal of the American Chemical Society*, **2021**, 143, 9123-9128	16.4	11
380	Assessment of interstitial potentials for rapid prediction of absolute band energies in crystals. *Journal of Chemical Physics*, **2021**, 155, 024113	3.9	0
379	Modeling Grain Boundaries in Polycrystalline Halide Perovskite Solar Cells. *Annual Review of Condensed Matter Physics*, **2021**, 12, 95-109	19.7	15
378	Multi-phonon proton transfer pathway in a molecular organic ferroelectric crystal. *Physical Chemistry Chemical Physics*, **2021**, 23, 2885-2890	3.6	2
377	Insights into the electric double-layer capacitance of two-dimensional electrically conductive metal-organic frameworks. *Journal of Materials Chemistry A*, **2021**, 9, 16006-16015	13	6
376	Perovskite-inspired materials for photovoltaics and beyond-from design to devices. *Nanotechnology*, **2021**, 32, 132004	3.4	47
375	Lead-free halide double perovskites: Toward stable and sustainable optoelectronic devices. *Materials Today*, **2021**,	21.8	16
374	Passivation Properties and Formation Mechanism of Amorphous Halide Perovskite Thin Films. *Advanced Functional Materials*, **2021**, 31, 2010330	15.6	4
373	Solvent engineered synthesis of layered SnO for high-performance anodes. *Npj 2D Materials and Applications*, **2021**, 5,	8.8	4
372	Phase Diagram and Cation Dynamics of Mixed MA1−xFAxPbBr3 Hybrid Perovskites. *Chemistry of Materials*, **2021**, 33, 5926-5934	9.6	6
371	Low Barrier for Exciton Self-Trapping Enables High Photoluminescence Quantum Yield in CsCuI. *Journal of Physical Chemistry Letters*, **2021**, 12, 8447-8452	6.4	6
370	Hidden spontaneous polarisation in the chalcohalide photovoltaic absorber SnSbSI. *Materials Horizons*, **2021**, 8, 2709-2716	14.4	8
369	Evolutionary exploration of polytypism in lead halide perovskites. *Chemical Science*, **2021**, 12, 12165-12173	9.4	4
368	Colloidal nano-MOFs nucleate and stabilize ultra-small quantum dots of lead bromide perovskites. *Chemical Science*, **2021**, 12, 6129-6135	9.4	4
367	Stabilized tilted-octahedra halide perovskites inhibit local formation of performance-limiting phases.. *Science*, **2021**, 374, 1598-1605	33.3	28

366	Hexagonal Stacking Faults Act as Hole-Blocking Layers in Lead Halide Perovskites. *ACS Energy Letters*, **2020**, 5, 2231-2233	20.1	8
365	Ligand engineering in Cu(II) paddle wheel metal□organic frameworks for enhanced semiconductivity. *Journal of Materials Chemistry A*, **2020**, 8, 13160-13165	13	6
364	Upper limit to the photovoltaic efficiency of imperfect crystals from first principles. *Energy and Environmental Science*, **2020**, 13, 1481-1491	35.4	58
363	Quick-start guide for first-principles modelling of point defects in crystalline materials. *JPhys Energy*, **2020**, 2, 036001	4.9	8
362	Polymorph exploration of bismuth stannate using first-principles phonon mode mapping.. *Chemical Science*, **2020**, 11, 7904-7909	9.4	2
361	Consensus statement for stability assessment and reporting for perovskite photovoltaics based on ISOS procedures. *Nature Energy*, **2020**, 5, 35-49	62.3	369
360	Sn 5s2 lone pairs and the electronic structure of tin sulphides: A photoreflectance, high-energy photoemission, and theoretical investigation. *Physical Review Materials*, **2020**, 4,	3.2	4
359	CarrierCapture.jl: Anharmonic Carrier Capture. *Journal of Open Source Software*, **2020**, 5, 2102	5.2	8
358	Low-cost descriptors of electrostatic and electronic contributions to anion redox activity in batteries. *IOP SciNotes*, **2020**, 1, 024805	1.2	3
357	Assessment of dynamic structural instabilities across 24 cubic inorganic halide perovskites. *Journal of Chemical Physics*, **2020**, 152, 024703	3.9	28
356	Descriptors for Electron and Hole Charge Carriers in Metal Oxides. *Journal of Physical Chemistry Letters*, **2020**, 11, 438-444	6.4	15
355	Bandgap lowering in mixed alloys of Cs2Ag(SbxBi1□)Br6 double perovskite thin films. *Journal of Materials Chemistry A*, **2020**, 8, 21780-21788	13	26
354	Suppression of phase transitions and glass phase signatures in mixed cation halide perovskites. *Nature Communications*, **2020**, 11, 5103	17.4	25
353	Manganese Porphyrin Interface Engineering in Perovskite Solar Cells. *ACS Applied Energy Materials*, **2020**, 3, 7353-7363	6.1	7
352	Modeling the dielectric constants of crystals using machine learning. *Journal of Chemical Physics*, **2020**, 153, 024503	3.9	12
351	Thermodynamic Stabilization of Mixed-Halide Perovskites against Phase Segregation. *Cell Reports Physical Science*, **2020**, 1, 100120	6.1	27
350	Probing the ionic defect landscape in halide perovskite solar cells. *Nature Communications*, **2020**, 11, 6098	17.4	32
349	Sustainable lead management in halide perovskite solar cells. *Nature Sustainability*, **2020**, 3, 1044-1051	22.1	40

348	Chemical Trends in the Lattice Thermal Conductivity of Li(Ni, Mn, Co)O2 (NMC) Battery Cathodes. *Chemistry of Materials*, **2020**, 32, 7542-7550	9.6	14
347	Anisotropic Electron Transport Limits Performance of Bi2WO6 Photoanodes. *Journal of Physical Chemistry C*, **2020**, 124, 18859-18867	3.8	3
346	Lattice Compression Increases the Activation Barrier for Phase Segregation in Mixed-Halide Perovskites. *ACS Energy Letters*, **2020**, 5, 3152-3158	20.1	37
345	A density functional theory study on the interface stability between CsPbBr3 and CuI. *AIP Advances*, **2020**, 10, 085023	1.5	1
344	The Holey Grail of Transparent Electronics. *Matter*, **2020**, 3, 604-606	12.7	2
343	Assessing the defect tolerance of kesterite-inspired solar absorbers. *Energy and Environmental Science*, **2020**, 13, 3489-3503	35.4	17
342	Crystal structure and metallization mechanism of the □adical metal. *Chemical Science*, **2020**, 11, 11699-11704	9.4	8
341	Performance-limiting nanoscale trap clusters at grain junctions in halide perovskites. *Nature*, **2020**, 580, 360-366	50.4	155
340	Data-Driven Discovery of Photoactive Quaternary Oxides Using First-Principles Machine Learning. *Chemistry of Materials*, **2019**, 31, 7221-7230	9.6	26
339	Highly Anisotropic Thermal Transport in LiCoO. *Journal of Physical Chemistry Letters*, **2019**, 10, 5552-5556	6.4	12
338	In situ observation of picosecond polaron self-localisation in □FeO photoelectrochemical cells. *Nature Communications*, **2019**, 10, 3962	17.4	52
337	Charge-transfer interactions between fullerenes and a mesoporous tetrathiafulvalene-based metal-organic framework. *Beilstein Journal of Nanotechnology*, **2019**, 10, 1883-1893	3	18
336	Room Temperature Metallic Conductivity in a Metal-Organic Framework Induced by Oxidation. *Journal of the American Chemical Society*, **2019**, 141, 16323-16330	16.4	49
335	Atomistic insights into the order□disorder transition in Cu2ZnSnS4 solar cells from Monte Carlo simulations. *Journal of Materials Chemistry A*, **2019**, 7, 312-321	13	14
334	Lattice strain causes non-radiative losses in halide perovskites. *Energy and Environmental Science*, **2019**, 12, 596-606	35.4	211
333	Lone-pair effect on carrier capture in Cu2ZnSnS4 solar cells. *Journal of Materials Chemistry A*, **2019**, 7, 2686-2693	13	33
332	Dielectric and ferroic properties of metal halide perovskites. *APL Materials*, **2019**, 7, 010901	5.7	108
331	Redox-active metal□organic frameworks for energy conversion and storage. *Journal of Materials Chemistry A*, **2019**, 7, 16571-16597	13	127

330	Emerging inorganic solar cell efficiency tables (Version 1). *JPhys Energy*, **2019**, 1, 032001	4.9	39
329	Effect of oxygen deficiency on the excited state kinetics of WO and implications for photocatalysis. *Chemical Science*, **2019**, 10, 5667-5677	9.4	56
328	Accumulation of Deep Traps at Grain Boundaries in Halide Perovskites. *ACS Energy Letters*, **2019**, 4, 1321-1327	20.2	76
327	Donor and acceptor characteristics of native point defects in GaN. *Journal Physics D: Applied Physics* , **2019**, 52, 335104	3	28
326	Vacancy-Driven Stabilization of the Cubic Perovskite Polymorph of CsPbI3. *Journal of Physical Chemistry C*, **2019**, 123, 9735-9744	3.8	32
325	Enhanced Charge Transport in 2D Perovskites via Fluorination of Organic Cation. *Journal of the American Chemical Society*, **2019**, 141, 5972-5979	16.4	170
324	Low-dimensional formamidinium lead perovskite architectures via controllable solvent intercalation. *Journal of Materials Chemistry C*, **2019**, 7, 3945-3951	7.1	15
323	Quick-start guide for first-principles modelling of semiconductor interfaces. *JPhys Energy*, **2019**, 1, 016001	4.9	7
322	Living in the salt-cocrystal continuum: indecisive organic complexes with thermochromic behaviour. *CrystEngComm*, **2019**, 21, 1626-1634	3.3	16
321	Finding a junction partner for candidate solar cell absorbers enargite and bournonite from electronic band and lattice matching. *Journal of Applied Physics*, **2019**, 125, 055703	2.5	13
320	Stability and flexibility of heterometallic formate perovskites with the dimethylammonium cation: pressure-induced phase transitions. *Physical Chemistry Chemical Physics*, **2019**, 21, 4200-4208	3.6	9
319	Impact of nonparabolic electronic band structure on the optical and transport properties of photovoltaic materials. *Physical Review B*, **2019**, 99,	3.3	33
318	Predicting synthesizability. *Journal Physics D: Applied Physics*, **2019**, 52,	3	161
317	Role of Electron–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	20.1	31
316	Intrinsic doping limit and defect-assisted luminescence in Cs4PbBr6. *Journal of Materials Chemistry A*, **2019**, 7, 20254-20261	13	33
315	Anharmonic lattice relaxation during nonradiative carrier capture. *Physical Review B*, **2019**, 100,	3.3	18
314	Status of materials and device modelling for kesterite solar cells. *JPhys Energy*, **2019**, 1, 042004	4.9	11
313	Heterostructure Engineering of a Reverse Water Gas Shift Photocatalyst. *Advanced Science*, **2019**, 6, 1902170	15.8	12

312	Crystal Engineering of Bi2WO6 to Polar Aurivillius-Phase Oxyhalides. *Journal of Physical Chemistry C* , **2019**, 123, 29155-29161	3.8	9
311	SMACT: Semiconducting Materials by Analogy and Chemical Theory. *Journal of Open Source Software*, **2019**, 4, 1361	5.2	10
310	CO2 Photoreduction: Heterostructure Engineering of a Reverse Water Gas Shift Photocatalyst (Adv. Sci. 22/2019). *Advanced Science*, **2019**, 6, 1970134	13.6	1
309	Identification of Lone-Pair Surface States on Indium Oxide. *Journal of Physical Chemistry C*, **2019**, 123, 1700-1709	3.8	16
308	Accelerated optimization of transparent, amorphous zinc-tin-oxide thin films for optoelectronic applications. *APL Materials*, **2019**, 7, 022509	5.7	12
307	Materials discovery by chemical analogy: role of oxidation states in structure prediction. *Faraday Discussions*, **2018**, 211, 553-568	3.6	14
306	Intrinsic Instability of the Hybrid Halide Perovskite Semiconductor CH 3 NH 3 PbI 3 *. *Chinese Physics Letters*, **2018**, 35, 036104	1.8	107
305	Vacancy defect configurations in the metal-organic framework UiO-66: energetics and electronic structure. *Journal of Materials Chemistry A*, **2018**, 6, 8507-8513	13	28
304	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
303	Identification of Killer Defects in Kesterite Thin-Film Solar Cells. *ACS Energy Letters*, **2018**, 3, 496-500	20.1	88
302	Point defect engineering in thin-film solar cells. *Nature Reviews Materials*, **2018**, 3, 194-210	73.3	176
301	Giant Electron-Phonon Coupling and Deep Conduction Band Resonance in Metal Halide Double Perovskite. *ACS Nano*, **2018**, 12, 8081-8090	16.7	123
300	Breathing-Dependent Redox Activity in a Tetrathiafulvalene-Based Metal-Organic Framework. *Journal of the American Chemical Society*, **2018**, 140, 10562-10569	16.4	48
299	Machine learning for molecular and materials science. *Nature*, **2018**, 559, 547-555	50.4	1282
298	Taking Control of Ion Transport in Halide Perovskite Solar Cells. *ACS Energy Letters*, **2018**, 3, 1983-1990	20.1	121
297	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, 193903	3.4	11
296	Dynamic symmetry breaking and spin splitting in metal halide perovskites. *Physical Review B*, **2018**, 98,	3.3	38
295	Heterometallic perovskite-type metal-organic framework with an ammonium cation: structure, phonons, and optical response of [NH]NaCrAl(HCOO) (x = 0, 0.025 and 0.5). *Physical Chemistry Chemical Physics*, **2018**, 20, 22284-22295	3.6	15

294	Opposing effects of stacking faults and antisite domain boundaries on the conduction band edge in kesterite quaternary semiconductors. *Physical Review Materials*, **2018**, 2,	3.2	12
293	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
292	Chapter 6:Computational Design of Photovoltaic Materials **2018**, 176-197		1
291	Computer-aided design of metal chalcohalide semiconductors: from chemical composition to crystal structure. *Chemical Science*, **2018**, 9, 1022-1030	9.4	35
290	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
289	Water oxidation catalysed by quantum-sized BiVO4. *Journal of Materials Chemistry A*, **2018**, 6, 24965-24970	13	7
288	Open-circuit voltage deficit in Cu2ZnSnS4 solar cells by interface bandgap narrowing. *Applied Physics Letters*, **2018**, 113, 212103	3.4	12
287	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
286	Oxidation states and ionicity. *Nature Materials*, **2018**, 17, 958-964	27	91
285	Hydrogen Bonding versus Entropy: Revealing the Underlying Thermodynamics of the Hybrid Organic–Inorganic Perovskite [CH3NH3]PbBr3. *Chemistry of Materials*, **2018**, 30, 8782-8788	9.6	19
284	Stability and electronic properties of planar defects in quaternary I2-II-IV-VI4 semiconductors. *Journal of Applied Physics*, **2018**, 124, 165705	2.5	5
283	Preface for Special Topic: Earth abundant materials in solar cells. *APL Materials*, **2018**, 6, 084401	5.7	2
282	An Unusual Phase Transition Driven by Vibrational Entropy Changes in a Hybrid Organic–Inorganic Perovskite. *Angewandte Chemie*, **2018**, 130, 9070-9074	3.6	4
281	An Unusual Phase Transition Driven by Vibrational Entropy Changes in a Hybrid Organic-Inorganic Perovskite. *Angewandte Chemie - International Edition*, **2018**, 57, 8932-8936	16.4	30
280	Prediction of multiband luminescence due to the gallium vacancy–oxygen defect complex in GaN. *Applied Physics Letters*, **2018**, 112, 262104	3.4	15
279	Perovskite-Inspired Photovoltaic Materials: Toward Best Practices in Materials Characterization and Calculations. *Chemistry of Materials*, **2017**, 29, 1964-1988	9.6	87
278	Self-Consistent Hybrid Functional Calculations: Implications for Structural, Electronic, and Optical Properties of Oxide Semiconductors. *Nanoscale Research Letters*, **2017**, 12, 19	5	31
277	The Steady Rise of Kesterite Solar Cells. *ACS Energy Letters*, **2017**, 2, 776-779	20.1	144

276	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
275	Chemical bonding at the metal organic framework/metal oxide interface: simulated epitaxial growth of MOF-5 on rutile TiO2. *Journal of Materials Chemistry A*, **2017**, 5, 6226-6232	13	15
274	Chemical and Lattice Stability of the Tin Sulfides. *Journal of Physical Chemistry C*, **2017**, 121, 6446-6454	3.8	52
273	Is iron unique in promoting electrical conductivity in MOFs?. *Chemical Science*, **2017**, 8, 4450-4457	9.4	106
272	DFT investigation into the underperformance of sulfide materials in photovoltaic applications. *Journal of Materials Chemistry A*, **2017**, 5, 9132-9140	13	16
271	Trimethylsulfonium Lead Triiodide: An Air-Stable Hybrid Halide Perovskite. *Inorganic Chemistry*, **2017**, 56, 6302-6309	5.1	35
270	Electron Counting in Solids: Oxidation States, Partial Charges, and Ionicity. *Journal of Physical Chemistry Letters*, **2017**, 8, 2074-2075	6.4	50
269	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
268	Vacuum-annealing induces sub-surface redox-states in surfactant-structured Fe2O3 photoanodes prepared by ink-jet printing. *Applied Catalysis B: Environmental*, **2017**, 211, 289-295	21.8	14
267	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
266	Designing porous electronic thin-film devices: band offsets and heteroepitaxy. *Faraday Discussions*, **2017**, 201, 207-219	3.6	26
265	Heterogeneous catalytic hydrogenation of CO by metal oxides: defect engineering - perfecting imperfection. *Chemical Society Reviews*, **2017**, 46, 4631-4644	58.5	212
264	Perspective: Theory and simulation of hybrid halide perovskites. *Journal of Chemical Physics*, **2017**, 146, 220901	3.9	87
263	Electroactive Nanoporous Metal Oxides and Chalcogenides by Chemical Design. *Chemistry of Materials*, **2017**, 29, 3663-3670	9.6	6
262	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
261	Metastable cubic tin sulfide: A novel phonon-stable chiral semiconductor. *APL Materials*, **2017**, 5, 036101	5.7	36
260	Theory of ionization potentials of nonmetallic solids. *Physical Review B*, **2017**, 95,	3.3	15
259	Indirect to direct bandgap transition in methylammonium lead halide perovskite. *Energy and Environmental Science*, **2017**, 10, 509-515	35.4	237

258	Quantifying Thermal Disorder in Metal-Organic Frameworks: Lattice Dynamics and Molecular Dynamics Simulations of Hybrid Formate Perovskites. *Journal of Physical Chemistry C*, **2017**, 121, 421-429	3.8	12
257	H-Center and V-Center Defects in Hybrid Halide Perovskites. *ACS Energy Letters*, **2017**, 2, 2713-2714	20.1	39
256	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
255	Slow Cooling of Hot Polarons in Halide Perovskite Solar Cells. *ACS Energy Letters*, **2017**, 2, 2647-2652	20.1	94
254	MOFs modeling and theory: general discussion. *Faraday Discussions*, **2017**, 201, 233-245	3.6	3
253	Electronic, magnetic and photophysical properties of MOFs and COFs: general discussion. *Faraday Discussions*, **2017**, 201, 87-99	3.6	5
252	New directions in gas sorption and separation with MOFs: general discussion. *Faraday Discussions*, **2017**, 201, 175-194	3.6	6
251	Catalysis in MOFs: general discussion. *Faraday Discussions*, **2017**, 201, 369-394	3.6	12
250	Anharmonic Origin of Giant Thermal Displacements in the Metal–Organic Framework UiO-67. *Journal of Physical Chemistry C*, **2017**, 121, 22010-22014	3.8	3
249	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
248	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	6.4	22
247	Electronic structure design for nanoporous, electrically conductive zeolitic imidazolate frameworks. *Journal of Materials Chemistry C*, **2017**, 5, 7726-7731	7.1	28
246	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	5.8	23
245	How Strong Is the Hydrogen Bond in Hybrid Perovskites?. *Journal of Physical Chemistry Letters*, **2017**, 8, 6154-6159	6.4	110
244	A rapidly-reversible absorptive and emissive vapochromic Pt(II) pincer-based chemical sensor. *Nature Communications*, **2017**, 8, 1800	17.4	56
243	Halide Perovskite Heteroepitaxy: Bond Formation and Carrier Confinement at the PbS–CsPbBr3 Interface. *Journal of Physical Chemistry C*, **2017**, 121, 27351-27356	3.8	32
242	Low-frequency optical phonon modes and carrier mobility in the halide perovskite CH3NH3PbBr3 using terahertz time-domain spectroscopy. *Applied Physics Letters*, **2017**, 111, 201903	3.4	38
241	Metallic Conductivity in a Two-Dimensional Cobalt Dithiolene Metal-Organic Framework. *Journal of the American Chemical Society*, **2017**, 139, 10863-10867	16.4	209

240	Instilling defect tolerance in new compounds. *Nature Materials*, **2017**,	27	156
239	Experimental and theoretical optical properties of methylammonium lead halide perovskites. *Nanoscale*, **2016**, 8, 6317-27	7.7	287
238	Correction: A universal chemical potential for sulfur vapours. *Chemical Science*, **2016**, 7, 6574	9.4	3
237	Anharmonicity in the High-Temperature Cmcm Phase of SnSe: Soft Modes and Three-Phonon Interactions. *Physical Review Letters*, **2016**, 117, 075502	7.4	104
236	Chemical principles for electroactive metal□rganic frameworks. *MRS Bulletin*, **2016**, 41, 870-876	3.2	34
235	Computational Screening of All Stoichiometric Inorganic Materials. *CheM*, **2016**, 1, 617-627	16.2	72
234	Organised chaos: entropy in hybrid inorganic-organic systems and other materials. *Chemical Science* , **2016**, 7, 6316-6324	9.4	49
233	Electronic Structure and Defect Physics of Tin Sulfides: SnS, Sn2S3, and SnS2. *Physical Review Applied*, **2016**, 6,	4.3	111
232	Analysis of electrostatic stability and ordering in quaternary perovskite solid solutions. *Physical Review B*, **2016**, 93,	3.3	8
231	Can Pb-Free Halide Double Perovskites Support High-Efficiency Solar Cells?. *ACS Energy Letters*, **2016**, 1, 949-955	20.1	301
230	Microscopic origin of entropy-driven polymorphism in hybrid organic-inorganic perovskite materials. *Physical Review B*, **2016**, 94,	3.3	39
229	Realistic Surface Descriptions of Heterometallic Interfaces: The Case of TiWC Coated in Noble Metals. *Journal of Physical Chemistry Letters*, **2016**, 7, 4475-4482	6.4	17
228	Electronic origins of photocatalytic activity in d0 metal organic frameworks. *Scientific Reports*, **2016** , 6, 23676	4.9	154
227	Ultrafast carrier dynamics in BiVO4 thin film photoanode material: interplay between free carriers, trapped carriers and low-frequency lattice vibrations. *Journal of Materials Chemistry A*, **2016**, 4, 18516-18523	10.7	45
226	One-dimensional Magnus-type platinum double salts. *Nature Communications*, **2016**, 7, 11950	17.4	27
225	A general forcefield for accurate phonon properties of metal-organic frameworks. *Physical Chemistry Chemical Physics*, **2016**, 18, 29316-29329	3.6	26
224	Frontier Orbital Engineering of Metal-Organic Frameworks with Extended Inorganic Connectivity: Porous Alkaline-Earth Oxides. *Inorganic Chemistry*, **2016**, 55, 7265-9	5.1	11
223	Lone-Pair Stabilization in Transparent Amorphous Tin Oxides: A Potential Route to p-Type Conduction Pathways. *Chemistry of Materials*, **2016**, 28, 4706-4713	9.6	26

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