

David O Scanlon

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

246
papers

13,882
citations

63
h-index

110
g-index

269
ext. papers

16,119
ext. citations

7.8
avg, IF

7
L-index

#	Paper	IF	Citations
246	Predicting Lithium Iron Oxysulfides for Battery Cathodes. <i>ACS Applied Energy Materials</i> , 2022 , 5, 575-584	6.1	0
245	Modulation of the Bi 6s Lone Pair State in Perovskites for High-Mobility p-Type Oxide Semiconductors.. <i>Advanced Science</i> , 2022 , e2104141	13.6	3
244	Understanding the Photocatalytic Activity of LaTiAgSO and LaTiCuSO for Green Hydrogen Production: Computational Insights.. <i>ACS Applied Energy Materials</i> , 2022 , 5, 1992-2001	6.1	1
243	Cation disorder engineering yields AgBiS ₂ nanocrystals with enhanced optical absorption for efficient ultrathin solar cells. <i>Nature Photonics</i> , 2022 , 16, 235-241	33.9	19
242	Deep UV transparent conductive oxide thin films realized through degenerately doped wide-bandgap gallium oxide. <i>Cell Reports Physical Science</i> , 2022 , 3, 100801	6.1	3
241	Machine learned calibrations to high-throughput molecular excited state calculations.. <i>Journal of Chemical Physics</i> , 2022 , 156, 134116	3.9	2
240	Ligand Field-Induced Exotic Dopant for Infrared Transparent Electrode: W in Rutile SnO ₂ . <i>Advanced Functional Materials</i> , 2022 , 32, 2110832	15.6	0
239	Enabling 100C Fast-Charging Bulk Bi Anodes for Na-Ion Batteries.. <i>Advanced Materials</i> , 2022 , e2201446	24	6
238	Extending the Performance Limit of Anodes: Insights from Diffusion Kinetics of Alloying Anodes. <i>Advanced Energy Materials</i> , 2021 , 11, 2003078	21.8	8
237	Enhanced visible light absorption in layered CsBiBr through mixed-valence Sn(ii)/Sn(iv) doping. <i>Chemical Science</i> , 2021 , 12, 14686-14699	9.4	8
236	Perspectives for next generation lithium-ion battery cathode materials. <i>APL Materials</i> , 2021 , 9, 109201	5.7	8
235	Experimental and Theoretical Study of the Electronic Structures of Lanthanide Indium Perovskites LnInO. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 6387-6400	3.8	3
234	Rapid Recombination by Cadmium Vacancies in CdTe. <i>ACS Energy Letters</i> , 2021 , 6, 1392-1398	20.1	12
233	Surfaxe: Systematic surface calculations. <i>Journal of Open Source Software</i> , 2021 , 6, 3171	5.2	2
232	Ab initio random structure searching for battery cathode materials. <i>Journal of Chemical Physics</i> , 2021 , 154, 174111	3.9	8
231	Electrochemical Oxidative Fluorination of an Oxide Perovskite. <i>Chemistry of Materials</i> , 2021 , 33, 5757-5768	9.8	2
230	2021 roadmap for sodium-ion batteries. <i>JPhys Energy</i> , 2021 , 3, 031503	4.9	24

229	Crystal Structure of Colloidally Prepared Metastable AgSe Nanocrystals. <i>Nano Letters</i> , 2021 , 21, 5881-5887	8.5	3
228	Surface Engineering Strategy Using Urea To Improve the Rate Performance of Na Ti O in Na-Ion Batteries. <i>Chemistry - A European Journal</i> , 2021 , 27, 3875-3886	4.8	6
227	Latest directions in p-type transparent conductor design. <i>Journal of Materials Chemistry C</i> , 2021 , 9, 11995-12009	5.1	5
226	Perovskite-inspired materials for photovoltaics and beyond-from design to devices. <i>Nanotechnology</i> , 2021 , 32, 132004	3.4	47
225	CaSbO and CaBiO: two promising mixed-anion thermoelectrics. <i>Journal of Materials Chemistry A</i> , 2021 , 9, 20417-20435	13	3
224	Accelerating the development of new solar absorbers by photoemission characterization coupled with density functional theory. <i>JPhys Energy</i> , 2021 , 3, 032001	4.9	1
223	Solvent engineered synthesis of layered SnO for high-performance anodes. <i>Npj 2D Materials and Applications</i> , 2021 , 5,	8.8	4
222	BaBi2O6: A Promising n-Type Thermoelectric Oxide with the PbSb2O6 Crystal Structure. <i>Chemistry of Materials</i> , 2021 , 33, 7441-7456	9.6	2
221	Hidden spontaneous polarisation in the chalcogenide photovoltaic absorber SnSbSI. <i>Materials Horizons</i> , 2021 , 8, 2709-2716	14.4	8
220	Accelerating cathode material discovery through ab initio random structure searching. <i>APL Materials</i> , 2021 , 9, 121111	5.7	3
219	Experimental and First-Principles Spectroscopy of CuSrSnS and CuBaSnS Photoabsorbers. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 50446-50454	9.5	5
218	Geometric Analysis and Formability of the Cubic A2BX6 Vacancy-Ordered Double Perovskite Structure. <i>Chemistry of Materials</i> , 2020 , 32, 9573-9583	9.6	15
217	Controlling the Thermoelectric Properties of Organometallic Coordination Polymers via Ligand Design. <i>Advanced Functional Materials</i> , 2020 , 30, 2003106	15.6	6
216	GeSe: Optical Spectroscopy and Theoretical Study of a van der Waals Solar Absorber. <i>Chemistry of Materials</i> , 2020 , 32, 3245-3253	9.6	19
215	Computational prediction of the thermoelectric performance of LaZnOPn (Pn = P, As). <i>Journal of Materials Chemistry A</i> , 2020 , 8, 7914-7924	13	6
214	Polymorph exploration of bismuth stannate using first-principles phonon mode mapping.. <i>Chemical Science</i> , 2020 , 11, 7904-7909	9.4	2
213	Resonant Ta Doping for Enhanced Mobility in Transparent Conducting SnO. <i>Chemistry of Materials</i> , 2020 , 32, 1964-1973	9.6	28
212	Enhanced Photocatalytic and Antibacterial Ability of Cu-Doped Anatase TiO Thin Films: Theory and Experiment. <i>ACS Applied Materials & Interfaces</i> , 2020 , 12, 15348-15361	9.5	49

211	Isotype Heterojunction Solar Cells Using n-Type Sb ₂ Se ₃ Thin Films. <i>Chemistry of Materials</i> , 2020 , 32, 2621-2630	34	
210	Assessing the limitations of transparent conducting oxides as thermoelectrics. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 11948-11957	13	9
209	Transition Metal Migration Can Facilitate Ionic Diffusion in Defect Garnet-Based Intercalation Electrodes. <i>ACS Energy Letters</i> , 2020 , 5, 1448-1455	20.1	3
208	Low-cost descriptors of electrostatic and electronic contributions to anion redox activity in batteries. <i>IOP SciNotes</i> , 2020 , 1, 024805	1.2	3
207	Native Defects and Their Doping Response in the Lithium Solid Electrolyte Li ₇ La ₃ Zr ₂ O ₁₂ . <i>Chemistry of Materials</i> , 2020 , 32, 1876-1886	9.6	15
206	Descriptors for Electron and Hole Charge Carriers in Metal Oxides. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 438-444	6.4	15
205	Bandgap lowering in mixed alloys of Cs ₂ Ag(SbxBi _{1-x})Br ₆ double perovskite thin films. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 21780-21788	13	26
204	Bi ₂ Sn ₂ O ₇ : a potential room temperature n-type oxide thermoelectric. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 16405-16420	13	10
203	Structure and Optical Properties of Layered Perovskite (MA) ₂ PbI ₂ Br(SCN) ₂ (0). <i>Inorganic Chemistry</i> , 2020 , 59, 17379-17384	5.1	2
202	Colloidal Synthesis and Optical Properties of Perovskite-Inspired Cesium Zirconium Halide Nanocrystals 2020 , 2, 1644-1652		23
201	Chemical Trends in the Lattice Thermal Conductivity of Li(Ni, Mn, Co)O ₂ (NMC) Battery Cathodes. <i>Chemistry of Materials</i> , 2020 , 32, 7542-7550	9.6	14
200	Computationally Driven Discovery of Layered Quinary Oxychalcogenides: Potential n-Type Transparent Conductors?. <i>Matter</i> , 2020 , 3, 759-781	12.7	5
199	Interaction of hydrogen with actinide dioxide (011) surfaces. <i>Journal of Chemical Physics</i> , 2020 , 153, 014705	39	1
198	Photocatalytic, structural and optical properties of mixed anion solid solutions Ba ₃ Sc _{2-x} In _x O ₅ Cu ₂ S ₂ and Ba ₃ In ₂ O ₅ Cu ₂ S _{2-y} Se _y . <i>Journal of Materials Chemistry A</i> , 2020 , 8, 19887-19897	13	5
197	Sb 5s ₂ lone pairs and band alignment of Sb ₂ Se ₃ : a photoemission and density functional theory study. <i>Journal of Materials Chemistry C</i> , 2020 , 8, 12615-12622	7.1	6
196	Resonant doping for high mobility transparent conductors: the case of Mo-doped In ₂ O ₃ . <i>Materials Horizons</i> , 2020 , 7, 236-243	14.4	30
195	Identifying Raman modes of Sb ₂ Se ₃ and their symmetries using angle-resolved polarised Raman spectra. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 8337-8344	13	25
194	Band edge evolution of transparent ZnM ₂ III ₂ O ₄ (MIII=Co, Rh, Ir) spinels. <i>Physical Review B</i> , 2019 , 100,	3.3	10

193	Highly Anisotropic Thermal Transport in LiCoO. <i>Journal of Physical Chemistry Letters</i> , 2019 , 10, 5552-5556.4	6.4	12
192	. <i>IEEE Journal of Photovoltaics</i> , 2019 , 9, 544-551	3.7	36
191	Magnetic structure of UO and NpO by first-principle methods. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 760-771	3.6	20
190	An experimental and theoretical study into NaSbS ₂ as an emerging solar absorber. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 2059-2067	7.1	13
189	Perspectives and Design Principles of Vacancy-Ordered Double Perovskite Halide Semiconductors. <i>Chemistry of Materials</i> , 2019 , 31, 1184-1195	9.6	89
188	Enhanced Li-ion dynamics in trivalently doped lithium phosphidosilicate Li ₂ SiP ₂ : a candidate material as a solid Li electrolyte. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 3953-3961	13	7
187	Origin of High-Efficiency Photoelectrochemical Water Splitting on Hematite/Functional Nanohybrid Metal Oxide Overlayer Photoanode after a Low Temperature Inert Gas Annealing Treatment. <i>ACS Omega</i> , 2019 , 4, 1449-1459	3.9	16
186	Donor and acceptor characteristics of native point defects in GaN. <i>Journal Physics D: Applied Physics</i> , 2019 , 52, 335104	3	28
185	Dispelling the Myth of Passivated Codoping in TiO. <i>Chemistry of Materials</i> , 2019 , 31, 2577-2589	9.6	12
184	Sensing and Discrimination of Explosives at Variable Concentrations with a Large-Pore MOF as Part of a Luminescent Array. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 11618-11626	9.5	35
183	Interaction of hydrogen with actinide dioxide (111) surfaces. <i>Journal of Chemical Physics</i> , 2019 , 150, 134701	9.1	4
182	The complex defect chemistry of antimony selenide. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 10739-10744	7.4	54
181	Two-dimensional eclipsed arrangement hybrid perovskites for tunable energy level alignments and photovoltaics. <i>Journal of Materials Chemistry C</i> , 2019 , 7, 5139-5147	7.1	14
180	Influence of One Specific Carbon-Carbon Bond on the Quality, Stability, and Photovoltaic Performance of Hybrid Organic-Inorganic Bismuth Iodide Materials. <i>ACS Applied Energy Materials</i> , 2019 , 2, 1579-1587	6.1	4
179	Exploiting Excited-State Aromaticity To Design Highly Stable Singlet Fission Materials. <i>Journal of the American Chemical Society</i> , 2019 , 141, 13867-13876	16.4	55
178	Intrinsic point defects and the n- and p-type dopability of the narrow gap semiconductors GaSb and InSb. <i>Physical Review B</i> , 2019 , 100,	3.3	8
177	Band Alignments, Band Gap, Core Levels, and Valence Band States in CuBiS for Photovoltaics. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 27033-27047	9.5	22
176	Anion Distribution, Structural Distortion, and Symmetry-Driven Optical Band Gap Bowing in Mixed Halide CsSnX Vacancy Ordered Double Perovskites. <i>Chemistry of Materials</i> , 2019 , 31, 9430-9444	9.6	32

175	Insights into the electronic structure of OsO ₂ using soft and hard x-ray photoelectron spectroscopy in combination with density functional theory. <i>Physical Review Materials</i> , 2019 , 3,	3.2	7
174	Electronic band structure and optical properties of boron arsenide. <i>Physical Review Materials</i> , 2019 , 3,	3.2	8
173	Anionic order and band gap engineering in vacancy ordered triple perovskites. <i>Chemical Communications</i> , 2019 , 55, 3164-3167	5.8	28
172	Leading the Charge of Electride Discovery. <i>Matter</i> , 2019 , 1, 1113-1114	12.7	0
171	Noncollinear Relativistic DFT + U Calculations of Actinide Dioxide Surfaces. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 356-366	3.8	11
170	Local corrugation and persistent charge density wave in ZrTe ₃ with Ni intercalation. <i>Physical Review B</i> , 2018 , 97,	3.3	12
169	Chemical Vapor Deposition of Photocatalytically Active Pure Brookite TiO ₂ Thin Films. <i>Chemistry of Materials</i> , 2018 , 30, 1353-1361	9.6	43
168	Deeper Understanding of Interstitial Boron-Doped Anatase Thin Films as A Multifunctional Layer Through Theory and Experiment. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 714-726	3.8	5
167	First-principles insights into tin-based two-dimensional hybrid halide perovskites for photovoltaics. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 5652-5660	13	50
166	Hidden magnetic order in plutonium dioxide nuclear fuel. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 20943-20951	3.6	20
165	Band gap temperature-dependence and exciton-like state in copper antimony sulphide, CuSbS ₂ . <i>APL Materials</i> , 2018 , 6, 084904	5.7	12
164	A novel laboratory-based hard X-ray photoelectron spectroscopy system. <i>Review of Scientific Instruments</i> , 2018 , 89, 073105	1.7	42
163	Phosphorus doped SnO thin films for transparent conducting oxide applications: synthesis, optoelectronic properties and computational models. <i>Chemical Science</i> , 2018 , 9, 7968-7980	9.4	27
162	Deep vs shallow nature of oxygen vacancies and consequent n-type carrier concentrations in transparent conducting oxides. <i>Physical Review Materials</i> , 2018 , 2,	3.2	46
161	Role of spin-orbit coupling in the electronic structure of IrO ₂ . <i>Physical Review Materials</i> , 2018 , 2,	3.2	9
160	sumo: Command-line tools for plotting and analysis of periodic ab initio calculations. <i>Journal of Open Source Software</i> , 2018 , 3, 717	5.2	127
159	Galore: Broadening and weighting for simulation of photoelectron spectroscopy. <i>Journal of Open Source Software</i> , 2018 , 3, 773	5.2	25
158	Anharmonicity and Octahedral Tilting in Hybrid Vacancy-Ordered Double Perovskites. <i>Chemistry of Materials</i> , 2018 , 30, 472-483	9.6	70

157	Oxidation states and ionicity. <i>Nature Materials</i> , 2018 , 17, 958-964	27	91
156	Correlated Polyhedral Rotations in the Absence of Polarons during Electrochemical Insertion of Lithium in ReO ₃ . <i>ACS Energy Letters</i> , 2018 , 3, 2513-2519	20.1	23
155	Preface for Special Topic: Earth abundant materials in solar cells. <i>APL Materials</i> , 2018 , 6, 084401	5.7	2
154	Tolerance Factor and Cooperative Tilting Effects in Vacancy-Ordered Double Perovskite Halides. <i>Chemistry of Materials</i> , 2018 , 30, 3909-3919	9.6	63
153	Defect Engineering of Earth-Abundant Solar Absorbers BiSI and BiSeI. <i>Chemistry of Materials</i> , 2018 , 30, 3827-3835	9.6	39
152	Enhanced electrical properties of antimony doped tin oxide thin films deposited via aerosol assisted chemical vapour deposition. <i>Journal of Materials Chemistry C</i> , 2018 , 6, 7257-7266	7.1	59
151	Self-Compensation in Transparent Conducting F-Doped SnO ₂ . <i>Advanced Functional Materials</i> , 2018 , 28, 1701900	15.6	56
150	Perovskite-Inspired Photovoltaic Materials: Toward Best Practices in Materials Characterization and Calculations. <i>Chemistry of Materials</i> , 2017 , 29, 1964-1988	9.6	87
149	Heterostructures of GaN with SiC and ZnO enhance carrier stability and separation in framework semiconductors. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2017 , 214, 1600440	1.6	6
148	Atypically small temperature-dependence of the direct band gap in the metastable semiconductor copper nitride Cu ₃ N. <i>Physical Review B</i> , 2017 , 95,	3.3	27
147	Chemical Vapor Deposition Synthesis and Optical Properties of NbO Thin Films with Hybrid Functional Theoretical Insight into the Band Structure and Band Gaps. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 18031-18038	9.5	36
146	Photocatalysis: Evidence and Effect of Photogenerated Charge Transfer for Enhanced Photocatalysis in WO ₃ /TiO ₂ Heterojunction Films: A Computational and Experimental Study (Adv. Funct. Mater. 18/2017). <i>Advanced Functional Materials</i> , 2017 , 27,	15.6	1
145	Electron Counting in Solids: Oxidation States, Partial Charges, and Ionicity. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 2074-2075	6.4	50
144	Demonstration of the donor characteristics of Si and O defects in GaN using hybrid QM/MM. <i>Physica Status Solidi (A) Applications and Materials Science</i> , 2017 , 214, 1600445	1.6	9
143	Exploring the PbS ₂ Bi ₂ S ₃ Series for Next Generation Energy Conversion Materials. <i>Chemistry of Materials</i> , 2017 , 29, 5156-5167	9.6	24
142	Evidence and Effect of Photogenerated Charge Transfer for Enhanced Photocatalysis in WO ₃ /TiO ₂ Heterojunction Films: A Computational and Experimental Study. <i>Advanced Functional Materials</i> , 2017 , 27, 1605413	15.6	76
141	Electroactive Nanoporous Metal Oxides and Chalcogenides by Chemical Design. <i>Chemistry of Materials</i> , 2017 , 29, 3663-3670	9.6	6
140	Electronic and defect properties of (CH ₃ NH ₃) ₂ Pb(SCN) ₂ I ₂ analogues for photovoltaic applications. <i>Journal of Materials Chemistry A</i> , 2017 , 5, 7845-7853	13	37

139	Computational and Experimental Study of Ta ₂ O ₅ Thin Films. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 202-210	3.8	17
138	The adsorption of Cu on the CeO(110) surface. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 27191-27203	3.6	14
137	Transparent conducting n-type ZnO:Sc synthesis, optoelectronic properties and theoretical insight. <i>Journal of Materials Chemistry C</i> , 2017 , 5, 7585-7597	7.1	38
136	Ising-like antiferromagnetism on the octahedral sublattice of a cobalt-containing garnet and the potential for quantum criticality. <i>Physical Review B</i> , 2017 , 95,	3.3	7
135	Narrow-band anisotropic electronic structure of ReS ₂ . <i>Physical Review B</i> , 2017 , 96,	3.3	33
134	Valence band modification of Cr ₂ O ₃ by Ni-doping: creating a high figure of merit p-type TCO. <i>Journal of Materials Chemistry C</i> , 2017 , 5, 12610-12618	7.1	24
133	Core Levels, Band Alignments, and Valence-Band States in CuSbS for Solar Cell Applications. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 41916-41926	9.5	40
132	Engineering Valence Band Dispersion for High Mobility p-Type Semiconductors. <i>Chemistry of Materials</i> , 2017 , 29, 2402-2413	9.6	47
131	Vibronic Structure in Room Temperature Photoluminescence of the Halide Perovskite CsBiBr. <i>Inorganic Chemistry</i> , 2017 , 56, 42-45	5.1	95
130	Stability of the M ₂ phase of vanadium dioxide induced by coherent epitaxial strain. <i>Physical Review B</i> , 2016 , 94,	3.3	51
129	Enhanced Photoresponse of FeS Films: The Role of Marcasite-Pyrite Phase Junctions. <i>Advanced Materials</i> , 2016 , 28, 9602-9607	24	53
128	A single-source precursor approach to solution processed indium arsenide thin films. <i>Journal of Materials Chemistry C</i> , 2016 , 4, 6761-6768	7.1	12
127	An assessment of silver copper sulfides for photovoltaic applications: theoretical and experimental insights. <i>Journal of Materials Chemistry A</i> , 2016 , 4, 12648-12657	13	32
126	Direct Observation of Electrostatically Driven Band Gap Renormalization in a Degenerate Perovskite Transparent Conducting Oxide. <i>Physical Review Letters</i> , 2016 , 116, 027602	7.4	83
125	Can Pb-Free Halide Double Perovskites Support High-Efficiency Solar Cells?. <i>ACS Energy Letters</i> , 2016 , 1, 949-955	20.1	301
124	Photoelectrochemistry: Enhanced Photoresponse of FeS ₂ Films: The Role of Marcasite/Pyrite Phase Junctions (Adv. Mater. 43/2016). <i>Advanced Materials</i> , 2016 , 28, 9656-9656	24	
123	Spatial Electron-hole Separation in a One Dimensional Hybrid Organic-Inorganic Lead Iodide. <i>Scientific Reports</i> , 2016 , 6, 20626	4.9	23
122	Modelling potential photovoltaic absorbers Cu ₃ MCh ₄ (M = V, Nb, Ta; Ch = S, Se, Te) using density functional theory. <i>Journal of Physics Condensed Matter</i> , 2016 , 28, 175801	1.8	10

121	Adsorption of formate species on Cu(h,k,l) low index surfaces. <i>Surface Science</i> , 2016 , 653, 45-54	1.8	19
120	Defect Tolerance to Intolerance in the Vacancy-Ordered Double Perovskite Semiconductors Cs ₂ SnI ₆ and Cs ₂ TeI ₆ . <i>Journal of the American Chemical Society</i> , 2016 , 138, 8453-64	16.4	264
119	n-Type doped transparent conducting binary oxides: an overview. <i>Journal of Materials Chemistry C</i> , 2016 , 4, 6946-6961	7.1	214
118	Relativistic electronic structure and band alignment of BiSI and BiSeI: candidate photovoltaic materials. <i>Journal of Materials Chemistry A</i> , 2016 , 4, 2060-2068	13	97
117	Lithium-ion conductivity in Li ₆ Y(BO ₃) ₃ : a thermally and electrochemically robust solid electrolyte. <i>Journal of Materials Chemistry A</i> , 2016 , 4, 6972-6979	13	9
116	Band gap and work function tailoring of SnO ₂ for improved transparent conducting ability in photovoltaics. <i>Journal of Materials Chemistry C</i> , 2016 , 4, 1467-1475	7.1	141
115	Interplay of Orbital and Relativistic Effects in Bismuth Oxyhalides: BiOF, BiOCl, BiOBr, and BiOI. <i>Chemistry of Materials</i> , 2016 , 28, 1980-1984	9.6	225
114	Assessing the potential of Mg-doped CrO ₂ as a novel p-type transparent conducting oxide. <i>Journal of Physics Condensed Matter</i> , 2016 , 28, 125501	1.8	16
113	Hybrid Organic-Inorganic Coordination Complexes as Tunable Optical Response Materials. <i>Inorganic Chemistry</i> , 2016 , 55, 3393-400	5.1	23
112	Bismuth oxyhalides: synthesis, structure and photoelectrochemical activity. <i>Chemical Science</i> , 2016 , 7, 4832-4841	9.4	197
111	Pilot-scale continuous synthesis of a vanadium-doped LiFePO ₄ /C nanocomposite high-rate cathodes for lithium-ion batteries. <i>Journal of Power Sources</i> , 2016 , 302, 410-418	8.9	51
110	Beyond methylammonium lead iodide: prospects for the emergent field of ns containing solar absorbers. <i>Chemical Communications</i> , 2016 , 53, 20-44	5.8	280
109	Quasi-particle electronic band structure and alignment of the V-VI-VII semiconductors SbSI, SbSBr, and SbSeI for solar cells. <i>Applied Physics Letters</i> , 2016 , 108, 112103	3.4	43
108	Band gap reduction in In _{Nx} Sb _{1-x} alloys: Optical absorption, k · P modeling, and density functional theory. <i>Applied Physics Letters</i> , 2016 , 109, 132104	3.4	9
107	On the application of the tolerance factor to inorganic and hybrid halide perovskites: a revised system. <i>Chemical Science</i> , 2016 , 7, 4548-4556	9.4	507
106	Single Step Solution Processed GaAs Thin Films from GaMe ₃ and tBuAsH ₂ under Ambient Pressure. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 7013-7019	3.8	10
105	Multifunctional P-Doped TiO ₂ Films: A New Approach to Self-Cleaning, Transparent Conducting Oxide Materials. <i>Chemistry of Materials</i> , 2015 , 27, 3234-3242	9.6	92
104	Electronic and surface properties of Ga-doped In ₂ O ₃ ceramics. <i>Applied Surface Science</i> , 2015 , 349, 970-987	27	25

103	Polymorph Engineering of TiO ₂ : Demonstrating How Absolute Reference Potentials Are Determined by Local Coordination. <i>Chemistry of Materials</i> , 2015 , 27, 3844-3851	9.6	92
102	Origin of High Mobility in Molybdenum-Doped Indium Oxide. <i>Chemistry of Materials</i> , 2015 , 27, 2788-2796	9.6	61
101	(CH ₃ NH ₃) ₂ Pb(SCN) ₂ I ₂ : a more stable structural motif for hybrid halide photovoltaics?. <i>Journal of Physical Chemistry Letters</i> , 2015 , 6, 4594-8	6.4	100
100	Structural, energetic and electronic properties of (100) surfaces for alkaline earth metal oxides as calculated with hybrid density functional theory. <i>Surface Science</i> , 2015 , 642, 58-65	1.8	16
99	Self-regulation mechanism for charged point defects in hybrid halide perovskites. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 1791-4	16.4	394
98	Scalable route to CH ₃ NH ₃ PbI ₃ perovskite thin films by aerosol assisted chemical vapour deposition. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 9071-9073	13	67
97	Band Gap Dependence on Cation Disorder in ZnSnN ₂ Solar Absorber. <i>Advanced Energy Materials</i> , 2015 , 5, 1501462	21.8	75
96	Antiferromagnetism at T>500K in the layered hexagonal ruthenate SrRu ₂ O ₆ . <i>Physical Review B</i> , 2015 , 92,	3.3	38
95	Buckeridge et al. Reply. <i>Physical Review Letters</i> , 2015 , 115, 029702	7.4	5
94	Band energy control of molybdenum oxide by surface hydration. <i>Applied Physics Letters</i> , 2015 , 107, 231605	9.4	23
93	Morphological Features and Band Bending at Nonpolar Surfaces of ZnO. <i>Journal of Physical Chemistry C</i> , 2015 , 119, 11598-11611	3.8	27
92	Interfacial Effects in Li _x VOPO ₄ and Evolution of the Electronic Structure. <i>Chemistry of Materials</i> , 2015 , 27, 8211-8219	9.6	33
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