David O Scanlon

List of Publications by Citations

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	Band alignment of rutile and anatase TiO. *Nature Materials*, **2013**, 12, 798-801	27	1656
245	On the application of the tolerance factor to inorganic and hybrid halide perovskites: a revised system. *Chemical Science*, **2016**, 7, 4548-4556	9.4	507
244	Theoretical and Experimental Study of the Electronic Structures of MoO3 and MoO2. *Journal of Physical Chemistry C*, **2010**, 114, 4636-4645	3.8	435
243	Self-regulation mechanism for charged point defects in hybrid halide perovskites. *Angewandte Chemie - International Edition*, **2015**, 54, 1791-4	16.4	394
242	Can Pb-Free Halide Double Perovskites Support High-Efficiency Solar Cells?. *ACS Energy Letters*, **2016**, 1, 949-955	20.1	301
241	Beyond methylammonium lead iodide: prospects for the emergent field of ns containing solar absorbers. *Chemical Communications*, **2016**, 53, 20-44	5.8	280
240	Defect Tolerance to Intolerance in the Vacancy-Ordered Double Perovskite Semiconductors Cs2SnI6 and Cs2TeI6. *Journal of the American Chemical Society*, **2016**, 138, 8453-64	16.4	264
239	Acceptor levels in p-type Cu(2)O: rationalizing theory and experiment. *Physical Review Letters*, **2009** , 103, 096405	7.4	237
238	Controlling bulk conductivity in topological insulators: key role of anti-site defects. *Advanced Materials*, **2012**, 24, 2154-8	24	227
237	Interplay of Orbital and Relativistic Effects in Bismuth Oxyhalides: BiOF, BiOCl, BiOBr, and BiOI. *Chemistry of Materials*, **2016**, 28, 1980-1984	9.6	225
236	n-Type doped transparent conducting binary oxides: an overview. *Journal of Materials Chemistry C*, **2016**, 4, 6946-6961	7.1	214
235	Bismuth oxyhalides: synthesis, structure and photoelectrochemical activity. *Chemical Science*, **2016**, 7, 4832-4841	9.4	197
234	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
233	Understanding the p-type defect chemistry of CuCrO2. *Journal of Materials Chemistry*, **2011**, 21, 3655		163
232	Role of Lattice Distortions in the Oxygen Storage Capacity of Divalently Doped CeO2. *Chemistry of Materials*, **2011**, 23, 4464-4468	9.6	158
231	Defect engineering of BaSnO3 for high-performance transparent conducting oxide applications. *Physical Review B*, **2013**, 87,	3.3	151
230	Sources of conductivity and doping limits in CdO from hybrid density functional theory. *Journal of the American Chemical Society*, **2011**, 133, 15065-72	16.4	149

229	Small polarons in Nb- and Ta-doped rutile and anatase TiO2. *Journal of Materials Chemistry*, **2009**, 19, 5175		143
228	Band gap and work function tailoring of SnO2 for improved transparent conducting ability in photovoltaics. *Journal of Materials Chemistry C*, **2016**, 4, 1467-1475	7.1	141
227	On the possibility of p-type SnO2. *Journal of Materials Chemistry*, **2012**, 22, 25236		134
226	sumo: Command-line tools for plotting and analysis of periodic ab initio calculations. *Journal of Open Source Software*, **2018**, 3, 717	5.2	127
225	Analysis of Intrinsic Defects in CeO2 Using a Koopmans-Like GGA+U Approach. *Journal of Physical Chemistry C*, **2012**, 116, 2443-2452	3.8	125
224	Modeling the polaronic nature of p-type defects in Cu2O: the failure of GGA and GGA + U. *Journal of Chemical Physics*, **2009**, 131, 124703	3.9	113
223	Undoped n-Type Cu2O: Fact or Fiction?. *Journal of Physical Chemistry Letters*, **2010**, 1, 2582-2585	6.4	111
222	Origin of the Bipolar Doping Behavior of SnO from X-ray Spectroscopy and Density Functional Theory. *Chemistry of Materials*, **2013**, 25, 3114-3123	9.6	107
221	Conductivity Limits in CuAlO2 from Screened-Hybrid Density Functional Theory. *Journal of Physical Chemistry Letters*, **2010**, 1, 3195-3199	6.4	102
220	Effect of Cr substitution on the electronic structure of CuAl1−xCrxO2. *Physical Review B*, **2009**, 79,	3.3	102
219	(CH3NH3)2Pb(SCN)2I2: a more stable structural motif for hybrid halide photovoltaics?. *Journal of Physical Chemistry Letters*, **2015**, 6, 4594-8	6.4	100
218	Bandgap engineering of ZnSnP2 for high-efficiency solar cells. *Applied Physics Letters*, **2012**, 100, 251911	3.4	99
217	Growth, disorder, and physical properties of ZnSnN2. *Applied Physics Letters*, **2013**, 103, 042109	3.4	98
216	Relativistic electronic structure and band alignment of BiSI and BiSeI: candidate photovoltaic materials. *Journal of Materials Chemistry A*, **2016**, 4, 2060-2068	13	97
215	Vibronic Structure in Room Temperature Photoluminescence of the Halide Perovskite CsBiBr. *Inorganic Chemistry*, **2017**, 56, 42-45	5.1	95
214	Understanding conductivity anomalies in Cu(I)-based delafossite transparent conducting oxides: Theoretical insights. *Journal of Chemical Physics*, **2010**, 132, 024707	3.9	93
213	Multifunctional P-Doped TiO2 Films: A New Approach to Self-Cleaning, Transparent Conducting Oxide Materials. *Chemistry of Materials*, **2015**, 27, 3234-3242	9.6	92
212	Polymorph Engineering of TiO2: Demonstrating How Absolute Reference Potentials Are Determined by Local Coordination. *Chemistry of Materials*, **2015**, 27, 3844-3851	9.6	92

211	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
210	Oxidation states and ionicity. *Nature Materials*, **2018**, 17, 958-964	27	91
209	Perspectives and Design Principles of Vacancy-Ordered Double Perovskite Halide Semiconductors. *Chemistry of Materials*, **2019**, 31, 1184-1195	9.6	89
208	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
207	Perovskite-Inspired Photovoltaic Materials: Toward Best Practices in Materials Characterization and Calculations. *Chemistry of Materials*, **2017**, 29, 1964-1988	9.6	87
206	Self-Regulation Mechanism for Charged Point Defects in Hybrid Halide Perovskites. *Angewandte Chemie*, **2015**, 127, 1811-1814	3.6	87
205	Geometry, Electronic Structure, and Bonding in CuMCh2(M = Sb, Bi; Ch = S, Se): Alternative Solar Cell Absorber Materials?. *Journal of Physical Chemistry C*, **2012**, 116, 7334-7340	3.8	87
204	Direct Observation of Electrostatically Driven Band Gap Renormalization in a Degenerate Perovskite Transparent Conducting Oxide. *Physical Review Letters*, **2016**, 116, 027602	7.4	83
203	Interface stoichiometry control to improve device voltage and modify band alignment in ZnO/Cu2O heterojunction solar cells. *Energy and Environmental Science*, **2014**, 7, 3606-3610	35.4	82
202	X-ray spectroscopic study of the electronic structure of CuCrO2. *Physical Review B*, **2009**, 79,	3.3	82
201	Solution Processing Route to Multifunctional Titania Thin Films: Highly Conductive and Photcatalytically Active Nb:TiO2. *Advanced Functional Materials*, **2014**, 24, 5075-5085	15.6	81
200	Understanding the electronic structure of IrO2 using hard-X-ray photoelectron spectroscopy and density-functional theory. *Physical Review Letters*, **2014**, 112, 117601	7.4	80
199	Tin Monoxide: Structural Prediction from First Principles Calculations with van der Waals Corrections. *Journal of Physical Chemistry C*, **2011**, 115, 19916-19924	3.8	79
198	Growth and properties of GaSbBi alloys. *Applied Physics Letters*, **2013**, 103, 142106	3.4	78
197	Convergence of density and hybrid functional defect calculations for compound semiconductors. *Physical Review B*, **2013**, 88,	3.3	77
196	Evidence and Effect of Photogenerated Charge Transfer for Enhanced Photocatalysis in WO3/TiO2 Heterojunction Films: A Computational and Experimental Study. *Advanced Functional Materials*, **2017**, 27, 1605413	15.6	76
195	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
194	Band Gap Dependence on Cation Disorder in ZnSnN2 Solar Absorber. *Advanced Energy Materials*, **2015**, 5, 1501462	21.8	75

193	La-doped BaSnO3: Degenerate perovskite transparent conducting oxide: Evidence from synchrotron x-ray spectroscopy. *Applied Physics Letters*, **2013**, 103, 042105	3.4	74
192	The origin of the enhanced oxygen storage capacity of Ce(1-x)(Pd/Pt)(x)O2. *Physical Chemistry Chemical Physics*, **2011**, 13, 4279-84	3.6	74
191	Anharmonicity and Octahedral Tilting in Hybrid Vacancy-Ordered Double Perovskites. *Chemistry of Materials*, **2018**, 30, 472-483	9.6	70
190	The electronic structure of the antimony chalcogenide series: Prospects for optoelectronic applications. *Journal of Solid State Chemistry*, **2014**, 213, 116-125	3.3	68
189	Scalable route to CH3NH3PbI3 perovskite thin films by aerosol assisted chemical vapour deposition. *Journal of Materials Chemistry A*, **2015**, 3, 9071-9073	13	67
188	(Cu2S2)(Sr3Sc2O5): A Layered, Direct Band Gap, p-Type Transparent Conducting Oxychalcogenide: A Theoretical Analysis.. *Chemistry of Materials*, **2009**, 21, 5435-5442	9.6	66
187	Electronic structure of mixed-valence silver oxide AgO from hybrid density-functional theory. *Physical Review B*, **2010**, 81,	3.3	64
186	The vapour phase detection of explosive markers and derivatives using two fluorescent metal–organic frameworks. *Journal of Materials Chemistry A*, **2015**, 3, 6351-6359	13	63
185	Reactivity on the (110) Surface of Ceria: A GGA+U Study of Surface Reduction and the Adsorption of CO and NO2. *Journal of Physical Chemistry C*, **2009**, 113, 11095-11103	3.8	63
184	Tolerance Factor and Cooperative Tilting Effects in Vacancy-Ordered Double Perovskite Halides. *Chemistry of Materials*, **2018**, 30, 3909-3919	9.6	63
183	Electronic Structures of Antimony Oxides. *Journal of Physical Chemistry C*, **2013**, 117, 14759-14769	3.8	62
182	Origin of High Mobility in Molybdenum-Doped Indium Oxide. *Chemistry of Materials*, **2015**, 27, 2788-2796	9.6	61
181	Elucidating the Nature of Pseudo Jahn–Teller Distortions in LixMnPO4: Combining Density Functional Theory with Soft and Hard X-ray Spectroscopy. *Journal of Physical Chemistry C*, **2013**, 117, 10383-10396	3.8	61
180	Band gap anomalies of the ZnM2(III)O4 (M(III)=Co, Rh, Ir) spinels. *Physical Chemistry Chemical Physics*, **2011**, 13, 9667-75	3.6	60
179	Understanding the defect chemistry of tin monoxide. *Journal of Materials Chemistry C*, **2013**, 1, 8194	7.1	59
178	Enhanced electrical properties of antimony doped tin oxide thin films deposited via aerosol assisted chemical vapour deposition. *Journal of Materials Chemistry C*, **2018**, 6, 7257-7266	7.1	59
177	Electron excess in alkaline earth sub-nitrides: 2D electron gas or 3D electride?. *Journal of Materials Chemistry C*, **2013**, 1, 3525	7.1	58
176	Cu3MCh3 (M = Sb, Bi; Ch = S, Se) as candidate solar cell absorbers: insights from theory. *Physical Chemistry Chemical Physics*, **2013**, 15, 15477-84	3.6	58

175	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
174	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
173	Self-Compensation in Transparent Conducting F-Doped SnO2. *Advanced Functional Materials*, **2018**, 28, 1701900	15.6	56
172	Exploiting Excited-State Aromaticity To Design Highly Stable Singlet Fission Materials. *Journal of the American Chemical Society*, **2019**, 141, 13867-13876	16.4	55
171	The complex defect chemistry of antimony selenide. *Journal of Materials Chemistry A*, **2019**, 7, 10739-10744	13	54
170	Enhanced Photoresponse of FeS Films: The Role of Marcasite-Pyrite Phase Junctions. *Advanced Materials*, **2016**, 28, 9602-9607	24	53
169	Stability of the M2 phase of vanadium dioxide induced by coherent epitaxial strain. *Physical Review B*, **2016**, 94,	3.3	51
168	Pilot-scale continuous synthesis of a vanadium-doped LiFePO4/C nanocomposite high-rate cathodes for lithium-ion batteries. *Journal of Power Sources*, **2016**, 302, 410-418	8.9	51
167	Electronic structures of silver oxides. *Physical Review B*, **2011**, 84,	3.3	51
166	Electron Counting in Solids: Oxidation States, Partial Charges, and Ionicity. *Journal of Physical Chemistry Letters*, **2017**, 8, 2074-2075	6.4	50
165	First-principles insights into tin-based two-dimensional hybrid halide perovskites for photovoltaics. *Journal of Materials Chemistry A*, **2018**, 6, 5652-5660	13	50
164	Valence-band density of states and surface electron accumulation in epitaxial SnO2 films. *Physical Review B*, **2014**, 90,	3.3	50
163	Enhanced Photocatalytic and Antibacterial Ability of Cu-Doped Anatase TiO Thin Films: Theory and Experiment. *ACS Applied Materials & Interfaces*, **2020**, 12, 15348-15361	9.5	49
162	The Nature of the Molybdenum Surface in Iron Molybdate. The Active Phase in Selective Methanol Oxidation. *Journal of Physical Chemistry C*, **2014**, 118, 26155-26161	3.8	49
161	Engineering Valence Band Dispersion for High Mobility p-Type Semiconductors. *Chemistry of Materials*, **2017**, 29, 2402-2413	9.6	47
160	Perovskite-inspired materials for photovoltaics and beyond-from design to devices. *Nanotechnology*, **2021**, 32, 132004	3.4	47
159	Uncovering the complex behavior of hydrogen in Cu2O. *Physical Review Letters*, **2011**, 106, 186403	7.4	46
158	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

157	Understanding doping anomalies in degenerate p-type semiconductor LaCuOSe. *Journal of Materials Chemistry C*, **2014**, 2, 3429-3438	7.1	45
156	Chemical Vapor Deposition of Photocatalytically Active Pure Brookite TiO2 Thin Films. *Chemistry of Materials*, **2018**, 30, 1353-1361	9.6	43
155	Quasi-particle electronic band structure and alignment of the V-VI-VII semiconductors SbSI, SbSBr, and SbSeI for solar cells. *Applied Physics Letters*, **2016**, 108, 112103	3.4	43
154	A novel laboratory-based hard X-ray photoelectron spectroscopy system. *Review of Scientific Instruments*, **2018**, 89, 073105	1.7	42
153	Chemical and structural indicators for large redox potentials in Fe-based positive electrode materials. *ACS Applied Materials & Interfaces*, **2014**, 6, 10832-9	9.5	40
152	Core Levels, Band Alignments, and Valence-Band States in CuSbS for Solar Cell Applications. *ACS Applied Materials & Interfaces*, **2017**, 9, 41916-41926	9.5	40
151	Understanding conductivity in SrCu2O2: stability, geometry and electronic structure of intrinsic defects from first principles. *Journal of Materials Chemistry*, **2010**, 20, 1086-1096		39
150	Defect Engineering of Earth-Abundant Solar Absorbers BiSI and BiSeI. *Chemistry of Materials*, **2018**, 30, 3827-3835	9.6	39
149	Dynamical response and instability in ceria under lattice expansion. *Physical Review B*, **2013**, 87,	3.3	38
148	Transparent conducting n-type ZnO:Sc synthesis, optoelectronic properties and theoretical insight. *Journal of Materials Chemistry C*, **2017**, 5, 7585-7597	7.1	38
147	Antiferromagnetism at T>500K in the layered hexagonal ruthenate SrRu2O6. *Physical Review B*, **2015**, 92,	3.3	38
146	Electronic and defect properties of (CH3NH3)2Pb(SCN)2I2 analogues for photovoltaic applications. *Journal of Materials Chemistry A*, **2017**, 5, 7845-7853	13	37
145	Electronic structure and band alignment of zinc nitride, Zn3N2. *RSC Advances*, **2014**, 4, 3306-3311	3.7	37
144	Nature of the band gap of Tl2O3. *Physical Review B*, **2011**, 83,	3.3	37
143	Chemical Vapor Deposition Synthesis and Optical Properties of NbO Thin Films with Hybrid Functional Theoretical Insight into the Band Structure and Band Gaps. *ACS Applied Materials & Interfaces*, **2017**, 9, 18031-18038	9.5	36
142	. *IEEE Journal of Photovoltaics*, **2019**, 9, 544-551	3.7	36
141	Sensing and Discrimination of Explosives at Variable Concentrations with a Large-Pore MOF as Part of a Luminescent Array. *ACS Applied Materials & Interfaces*, **2019**, 11, 11618-11626	9.5	35
140	Isotype Heterojunction Solar Cells Using n-Type Sb2Se3 Thin Films. *Chemistry of Materials*, **2020**, 32, 2621-2630	9.6	34

139	Interlayer cation exchange stabilizes polar perovskite surfaces. *Advanced Materials*, **2014**, 26, 7252-6	24	34
138	Intrinsic ferromagnetism in CeO(2): dispelling the myth of vacancy site localization mediated superexchange. *Journal of Physics Condensed Matter*, **2009**, 21, 405502	1.8	34
137	Narrow-band anisotropic electronic structure of ReS2. *Physical Review B*, **2017**, 96,	3.3	33
136	Interfacial Effects in □LixVOPO4 and Evolution of the Electronic Structure. *Chemistry of Materials*, **2015**, 27, 8211-8219	9.6	33
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134	Combinatorial Atmospheric Pressure Chemical Vapor Deposition of F:TiO2; the Relationship between Photocatalysis and Transparent Conducting Oxide Properties. *Advanced Functional Materials*, **2014**, 24, 1758-1771	15.6	33
133	Comparative study of bandwidths in copper delafossites from x-ray emission spectroscopy. *Physical Review B*, **2009**, 80,	3.3	33
132	An assessment of silver copper sulfides for photovoltaic applications: theoretical and experimental insights. *Journal of Materials Chemistry A*, **2016**, 4, 12648-12657	13	32
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128	Resonant doping for high mobility transparent conductors: the case of Mo-doped In2O3. *Materials Horizons*, **2020**, 7, 236-243	14.4	30
127	Donor and acceptor characteristics of native point defects in GaN. *Journal Physics D: Applied Physics* , **2019**, 52, 335104	3	28
126	Resonant Ta Doping for Enhanced Mobility in Transparent Conducting SnO. *Chemistry of Materials*, **2020**, 32, 1964-1973	9.6	28
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123	Atypically small temperature-dependence of the direct band gap in the metastable semiconductor copper nitride Cu3N. *Physical Review B*, **2017**, 95,	3.3	27
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121	Understanding the defect chemistry of alkali metal strontium silicate solid solutions: insights from experiment and theory. *Journal of Materials Chemistry A*, **2014**, 2, 17919-17924	13	27
120	Morphological Features and Band Bending at Nonpolar Surfaces of ZnO. *Journal of Physical Chemistry C*, **2015**, 119, 11598-11611	3.8	27
119	Bandgap lowering in mixed alloys of Cs2Ag(SbxBi1-x)Br6 double perovskite thin films. *Journal of Materials Chemistry A*, **2020**, 8, 21780-21788	13	26
118	Electronic and surface properties of Ga-doped In2O3 ceramics. *Applied Surface Science*, **2015**, 349, 970-982	6.7	25
117	The nature of oxygen states on the surfaces of CeO2 and La-doped CeO2. *Chemical Physics Letters*, **2014**, 608, 239-243	2.5	25
116	Galore: Broadening and weighting for simulation of photoelectron spectroscopy. *Journal of Open Source Software*, **2018**, 3, 773	5.2	25
115	Identifying Raman modes of Sb2Se3 and their symmetries using angle-resolved polarised Raman spectra. *Journal of Materials Chemistry A*, **2020**, 8, 8337-8344	13	25
114	Exploring the PbS-Bi2S3 Series for Next Generation Energy Conversion Materials. *Chemistry of Materials*, **2017**, 29, 5156-5167	9.6	24
113	Valence band modification of Cr2O3 by Ni-doping: creating a high figure of merit p-type TCO. *Journal of Materials Chemistry C*, **2017**, 5, 12610-12618	7.1	24
112	The Use of the “+U” Correction in Describing Defect States at Metal Oxide Surfaces: Oxygen Vacancies on CeO2 and TiO2, and Li-doping of MgO. *E-Journal of Surface Science and Nanotechnology*, **2009**, 7, 389-394	0.7	24
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110	Spatial Electron-hole Separation in a One Dimensional Hybrid Organic-Inorganic Lead Iodide. *Scientific Reports*, **2016**, 6, 20626	4.9	23
109	Hybrid Organic-Inorganic Coordination Complexes as Tunable Optical Response Materials. *Inorganic Chemistry*, **2016**, 55, 3393-400	5.1	23
108	PbO2: from semi-metal to transparent conducting oxide by defect chemistry control. *Chemical Communications*, **2013**, 49, 448-50	5.8	23
107	Band energy control of molybdenum oxide by surface hydration. *Applied Physics Letters*, **2015**, 107, 231605	3.4	23
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105	Comparison of the defective pyrochlore and ilmenite polymorphs of AgSbO3 using GGA and hybrid DFT. *Physical Review B*, **2011**, 83,	3.3	23
104	Colloidal Synthesis and Optical Properties of Perovskite-Inspired Cesium Zirconium Halide Nanocrystals **2020**, 2, 1644-1652		23

103	Correlated Polyhedral Rotations in the Absence of Polarons during Electrochemical Insertion of Lithium in ReO3. *ACS Energy Letters*, **2018**, 3, 2513-2519	20.1	23
102	Band Alignments, Band Gap, Core Levels, and Valence Band States in CuBiS for Photovoltaics. *ACS Applied Materials & Interfaces*, **2019**, 11, 27033-27047	9.5	22
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96	Adsorption of formate species on Cu(h,k,l) low index surfaces. *Surface Science*, **2016**, 653, 45-54	1.8	19
95	Understanding the stability of MnPO4. *Journal of Materials Chemistry A*, **2014**, 2, 12827	13	19
94	Cation disorder engineering yields AgBiS2 nanocrystals with enhanced optical absorption for efficient ultrathin solar cells. *Nature Photonics*, **2022**, 16, 235-241	33.9	19
93	The electronic structure of silver orthophosphate: experiment and theory. *Journal of Materials Chemistry A*, **2014**, 2, 6092-6099	13	18
92	Band gap engineering of In2O3 by alloying with Tl2O3. *Applied Physics Letters*, **2013**, 103, 262108	3.4	18
91	Computational and Experimental Study of Ta2O5 Thin Films. *Journal of Physical Chemistry C*, **2017**, 121, 202-210	3.8	17
90	Polymorphism of indium oxide: Materials physics of orthorhombic In2O3. *Physical Review B*, **2013**, 88,	3.3	17
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87	Structural, energetic and electronic properties of (100) surfaces for alkaline earth metal oxides as calculated with hybrid density functional theory. *Surface Science*, **2015**, 642, 58-65	1.8	16
86	Assessing the potential of Mg-doped CrO as a novel p-type transparent conducting oxide. *Journal of Physics Condensed Matter*, **2016**, 28, 125501	1.8	16

85	Geometric Analysis and Formability of the Cubic A2BX6 Vacancy-Ordered Double Perovskite Structure. *Chemistry of Materials*, **2020**, 32, 9573-9583	9.6	15
84	Native Defects and Their Doping Response in the Lithium Solid Electrolyte Li7La3Zr2O12. *Chemistry of Materials*, **2020**, 32, 1876-1886	9.6	15
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80	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
79	An experimental and theoretical study into NaSbS2 as an emerging solar absorber. *Journal of Materials Chemistry C*, **2019**, 7, 2059-2067	7.1	13
78	Stability, geometry, and electronic structure of an alternative I-III-VI2 material, CuScS2: A hybrid density functional theory analysis. *Applied Physics Letters*, **2010**, 97, 131904	3.4	13
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