

M Saiful Islam

List of Publications by Year in descending order

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139
papers

17,951
citations

13865

67
h-index

14208

128
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all docs

143
docs citations

143
times ranked

18275
citing authors

#	ARTICLE	IF	CITATIONS
1	Ionic transport in hybrid lead iodide perovskite solar cells. <i>Nature Communications</i> , 2015, 6, 7497.	12.8	2,154
2	Fundamentals of inorganic solid-state electrolytes for batteries. <i>Nature Materials</i> , 2019, 18, 1278-1291.	27.5	1,341
3	Atomic-Scale Investigation of Defects, Dopants, and Lithium Transport in the LiFePO ₄ Olivine-Type Battery Material. <i>Chemistry of Materials</i> , 2005, 17, 5085-5092.	6.7	966
4	Fast oxygen diffusion and iodide defects mediate oxygen-induced degradation of perovskite solar cells. <i>Nature Communications</i> , 2017, 8, 15218.	12.8	917
5	Lithium and sodium battery cathode materials: computational insights into voltage, diffusion and nanostructural properties. <i>Chemical Society Reviews</i> , 2014, 43, 185-204.	38.1	899
6	Lithium Battery Materials Li _M PO ₄ (M = Mn, Fe, Co, and Ni): Insights into Defect Association, Transport Mechanisms, and Doping Behavior. <i>Chemistry of Materials</i> , 2008, 20, 5907-5915.	6.7	483
7	Ionic transport in ABO ₃ perovskite oxides: a computer modelling tour. <i>Journal of Materials Chemistry</i> , 2000, 10, 1027-1038.	6.7	453
8	Silicate cathodes for lithium batteries: alternatives to phosphates?. <i>Journal of Materials Chemistry</i> , 2011, 21, 9811.	6.7	310
9	Structure and Lithium Transport Pathways in Li ₂ FeSiO ₄ Cathodes for Lithium Batteries. <i>Journal of the American Chemical Society</i> , 2011, 133, 13031-13035.	13.7	277
10	The lithium intercalation process in the low-voltage lithium battery anode Li _{1+x} V _{1-x} O ₂ . <i>Nature Materials</i> , 2011, 10, 223-229.	27.5	267
11	Defect chemistry and oxygen ion migration in the apatite-type materials La _{9.33} Si ₆ O ₂₆ and La ₈ Sr ₂ Si ₆ O ₂₆ . <i>Journal of Materials Chemistry</i> , 2003, 13, 1956.	6.7	250
12	Computer Simulation Studies of Bulk Reduction and Oxygen Migration in CeO ₂ -ZrO ₂ Solid Solutions. <i>Journal of Physical Chemistry B</i> , 1997, 101, 1750-1753.	2.6	240
13	Developing apatites for solid oxide fuel cells: insight into structural, transport and doping properties. <i>Journal of Materials Chemistry</i> , 2007, 17, 3104.	6.7	239
14	Degradation mechanism of hybrid tin-based perovskite solar cells and the critical role of tin (IV) iodide. <i>Nature Communications</i> , 2021, 12, 2853.	12.8	236
15	Surface structures and crystal morphologies of LiFePO ₄ : relevance to electrochemical behaviour. <i>Journal of Materials Chemistry</i> , 2008, 18, 1209.	6.7	232
16	Na-ion mobility in layered Na ₂ FePO ₄ F and olivine Na[Fe,Mn]PO ₄ . <i>Energy and Environmental Science</i> , 2013, 6, 2257.	30.8	228
17	Atomic-Scale Influence of Grain Boundaries on Li-Ion Conduction in Solid Electrolytes for All-Solid-State Batteries. <i>Journal of the American Chemical Society</i> , 2018, 140, 362-368.	13.7	226
18	Structural and Mechanistic Insights into Fast Lithium-Ion Conduction in Li ₄ SiO ₄ Li ₃ PO ₄ Solid Electrolytes. <i>Journal of the American Chemical Society</i> , 2015, 137, 9136-9145.	13.7	223

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19	Lithium Extraction Mechanism in Li-Rich Li_2MnO_3 Involving Oxygen Hole Formation and Dimerization. <i>Chemistry of Materials</i> , 2016, 28, 6656-6663.	6.7	210
20	Surface and Reduction Energetics of the $\text{CeO}_2\text{-ZrO}_2$ Catalysts. <i>Journal of Physical Chemistry B</i> , 1998, 102, 557-561.	2.6	208
21	Water Adsorption and Its Effect on the Stability of Low Index Stoichiometric and Reduced Surfaces of Ceria. <i>Journal of Physical Chemistry C</i> , 2012, 116, 7073-7082.	3.1	204
22	Rutile $(\sqrt{2})\text{MnO}_2$ Surfaces and Vacancy Formation for High Electrochemical and Catalytic Performance. <i>Journal of the American Chemical Society</i> , 2014, 136, 1418-1426.	13.7	186
23	The influence of large cations on the electrochemical properties of tunnel-structured metal oxides. <i>Nature Communications</i> , 2016, 7, 13374.	12.8	180
24	Electrochemistry of Hollandite $\text{Li}_x\text{-MnO}_2$: Li-Ion and Na-Ion Insertion and Li_2O Incorporation. <i>Chemistry of Materials</i> , 2013, 25, 2515-2526.	6.7	172
25	Lithium Insertion and Transport in the $\text{TiO}_2\text{-B}$ Anode Material: A Computational Study. <i>Chemistry of Materials</i> , 2009, 21, 4778-4783.	6.7	169
26	Partial cation substitution reduces iodide ion transport in lead iodide perovskite solar cells. <i>Energy and Environmental Science</i> , 2019, 12, 2264-2272.	30.8	168
27	$\text{Li}_2\text{MnSiO}_4$ Lithium Battery Material: Atomic-Scale Study of Defects, Lithium Mobility, and Trivalent Dopants. <i>Chemistry of Materials</i> , 2009, 21, 5196-5202.	6.7	160
28	Bulk Reduction and Oxygen Migration in the Ceria-Based Oxides. <i>Chemistry of Materials</i> , 2000, 12, 677-681.	6.7	157
29	Alkali-ion Conduction Paths in LiFeSO_4F and NaFeSO_4F avorite-Type Cathode Materials. <i>Chemistry of Materials</i> , 2011, 23, 2278-2284.	6.7	156
30	The Impact of Atmosphere on the Local Luminescence Properties of Metal Halide Perovskite Grains. <i>Advanced Materials</i> , 2018, 30, e1706208.	21.0	149
31	High voltage structural evolution and enhanced Na-ion diffusion in $\text{P2-Na}_{2/3}\text{Ni}_{1/3}\text{Mg}_x\text{Mn}_{2/3}\text{O}_2$ (0 $\leq x < 1$). <i>Environmental Science</i> . 2018, 11, 1470-1479.	30.8	148
32	Enhancing the Lithium Ion Conductivity in Lithium Superionic Conductor (LISICON) Solid Electrolytes through a Mixed Polyanion Effect. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 7050-7058.	8.0	147
33	Defect chemistry and proton-dopant association in BaZrO_3 and BaPrO_3 . <i>Journal of Materials Chemistry</i> , 2010, 20, 6258.	6.7	145
34	Dopant Substitution and Ion Migration in the LaGaO_3 -Based Oxygen Ion Conductor. <i>Journal of Physical Chemistry B</i> , 1998, 102, 3099-3104.	2.6	142
35	Proton Migration and Defect Interactions in the CaZrO_3 Orthorhombic Perovskite: A Quantum Mechanical Study. <i>Chemistry of Materials</i> , 2001, 13, 2049-2055.	6.7	142
36	Anti-Site Defects and Ion Migration in the $\text{LiFe}_{0.5}\text{Mn}_{0.5}\text{PO}_4$ Mixed-Metal Cathode Material. <i>Chemistry of Materials</i> , 2010, 22, 1242-1248.	6.7	140

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37	A review of structural properties and synthesis methods of solid electrolyte materials in the Li ₂ S- $\hat{\sim}$ P2S ₅ binary system. Journal of Power Sources, 2018, 407, 31-43.	7.8	140
38	Insights into Changes in Voltage and Structure of Li ₂ FeSiO ₄ Polymorphs for Lithium-Ion Batteries. Chemistry of Materials, 2012, 24, 2155-2161.	6.7	128
39	An apatite for fast oxide ion conduction Electronic supplementary information (ESI) available: interatomic potentials. See http://www.rsc.org/suppdata/cc/b3/b301179h/ . Chemical Communications, 2003, , 1486.	4.1	127
40	Mixed A-Cation Perovskites for Solar Cells: Atomic-Scale Insights Into Structural Distortion, Hydrogen Bonding, and Electronic Properties. Chemistry of Materials, 2018, 30, 5194-5204.	6.7	127
41	Good Vibrations: Locking of Octahedral Tilting in Mixed-Cation Iodide Perovskites for Solar Cells. ACS Energy Letters, 2017, 2, 2424-2429.	17.4	126
42	Surface properties of $\hat{\pm}$ -MnO ₂ : relevance to catalytic and supercapacitor behaviour. Journal of Materials Chemistry A, 2014, 2, 15509-15518.	10.3	121
43	Sodium Ion Diffusion and Voltage Trends in Phosphates Na ₄ M ₃ (PO ₄) ₂ P ₂ O ₇ (M = Fe, Tj ETQq1 1 0.784614 rgBT	10.1	114
44	Defect chemistry and lithium-ion migration in polymorphs of the cathode material Li ₂ MnSiO ₄ . Journal of Materials Chemistry A, 2013, 1, 4207.	10.3	113
45	Mechanisms of Lithium Intercalation and Conversion Processes in Organic-Inorganic Halide Perovskites. ACS Energy Letters, 2017, 2, 1818-1824.	17.4	111
46	Crystal Structures, Local Atomic Environments, and Ion Diffusion Mechanisms of Scandium-Substituted Sodium Superionic Conductor (NASICON) Solid Electrolytes. Chemistry of Materials, 2018, 30, 2618-2630.	6.7	109
47	Defect chemistry and surface properties of LaCoO ₃ . Journal of Materials Chemistry, 2000, 10, 2298-2305.	6.7	107
48	Doping and defect association in AZrO ₃ (A = Ca, Ba) and LaMO ₃ (M = Sc, Ga) perovskite-type ionic conductors. Dalton Transactions, 2004, , 3061.	3.3	106
49	Lithium Coordination Sites in Li _x TiO ₂ (B): A Structural and Computational Study. Chemistry of Materials, 2010, 22, 6426-6432.	6.7	104
50	Lead-Free Perovskite Semiconductors Based on Germanium-Tin Solid Solutions: Structural and Optoelectronic Properties. Journal of Physical Chemistry C, 2018, 122, 5940-5947.	3.1	104
51	Fluid-enhanced surface diffusion controls intraparticle phase transformations. Nature Materials, 2018, 17, 915-922.	27.5	104
52	Phase Behavior and Polymorphism of Formamidinium Lead Iodide. Chemistry of Materials, 2018, 30, 3768-3778.	6.7	104
53	Atomic-Scale Insight into LaFeO ₃ Perovskite: Defect Nanoclusters and Ion Migration. Journal of Physical Chemistry C, 2008, 112, 4455-4462.	3.1	100
54	Nanostructuring of $\hat{\pm}$ -MnO ₂ : The Important Role of Surface to Bulk Ion Migration. Chemistry of Materials, 2013, 25, 536-541.	6.7	99

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55	Atomistic Simulation Studies of Lithium and Proton Insertion in Spinel Lithium Manganates. Journal of Physical Chemistry B, 1997, 101, 8156-8163.	2.6	98
56	Atomistic study of dopant site-selectivity and defect association in the lanthanum gallate perovskite. Journal of Materials Chemistry, 2004, 14, 86.	6.7	96
57	Elucidating lithium-ion and proton dynamics in anti-perovskite solid electrolytes. Energy and Environmental Science, 2018, 11, 2993-3002.	30.8	95
58	Sodium-ion battery cathodes $\text{Na}_2\text{FeP}_2\text{O}_7$ and $\text{Na}_2\text{MnP}_2\text{O}_7$: diffusion behaviour for high rate performance. Journal of Materials Chemistry A, 2014, 2, 11807-11812.	10.3	92
59	Complete structural model for lanthanum tungstate: a chemically stable high temperature proton conductor by means of intrinsic defects. Journal of Materials Chemistry, 2012, 22, 1762-1764.	6.7	91
60	Understanding the stability of mixed A-cation lead iodide perovskites. Journal of Materials Chemistry A, 2017, 5, 22495-22499.	10.3	91
61	Toward Understanding the Different Influences of Grain Boundaries on Ion Transport in Sulfide and Oxide Solid Electrolytes. Chemistry of Materials, 2019, 31, 5296-5304.	6.7	89
62	Putting the Squeeze on Lead Iodide Perovskites: Pressure-Induced Effects To Tune Their Structural and Optoelectronic Behavior. Chemistry of Materials, 2019, 31, 4063-4071.	6.7	87
63	Reduction Process in $\text{CeO}_2 \sim \text{MO}$ and $\text{CeO}_2 \sim \text{M}_2\text{O}_3$ Mixed Oxides: A Computer Simulation Study. Chemistry of Materials, 2003, 15, 3781-3785.	6.7	82
64	Particle Morphology and Lithium Segregation to Surfaces of the $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ Solid Electrolyte. Chemistry of Materials, 2018, 30, 3019-3027.	6.7	80
65	Redox Chemistry and the Role of Trapped Molecular O_2 in Li-Rich Disordered Rocksalt Oxyfluoride Cathodes. Journal of the American Chemical Society, 2020, 142, 21799-21809.	13.7	77
66	Surface structures and defect properties of pure and doped La_2NiO_4 . Journal of Materials Chemistry, 2001, 11, 2597-2602.	6.7	75
67	A comparison of the effect of rare earth vs Si site doping on the conductivities of apatite-type rare earth silicates. Journal of Solid State Electrochemistry, 2006, 10, 562-568.	2.5	72
68	$\text{Na}_2\text{CoSiO}_4$ as a cathode material for sodium-ion batteries: structure, electrochemistry and diffusion pathways. Physical Chemistry Chemical Physics, 2016, 18, 32744-32752.	2.8	69
69	Atomistic Insights into the Oriented Attachment of Tunnel-Based Oxide Nanostructures. ACS Nano, 2016, 10, 539-548.	14.6	66
70	Depth-dependent oxygen redox activity in lithium-rich layered oxide cathodes. Journal of Materials Chemistry A, 2019, 7, 25355-25368.	10.3	62
71	Defects, Dopants, and Protons in LaNbO_4 . Chemistry of Materials, 2010, 22, 5912-5917.	6.7	59
72	Feeling the strain: enhancing ionic transport in olivine phosphate cathodes for Li- and Na-ion batteries through strain effects. Journal of Materials Chemistry A, 2016, 4, 6998-7004.	10.3	59

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73	Composition Screening of Lithium- and Sodium-Rich Anti-Perovskites for Fast-Conducting Solid Electrolytes. <i>Journal of Physical Chemistry C</i> , 2018, 122, 23978-23984.	3.1	59
74	Under Pressure: Mechanochemical Effects on Structure and Ion Conduction in the Sodium-Ion Solid Electrolyte Na_3PS_4 . <i>Journal of the American Chemical Society</i> , 2020, 142, 18422-18436.	13.7	58
75	High voltage sulphate cathodes $\text{Li}_2\text{M}(\text{SO}_4)_2$ (M = Fe, Mn, Co): atomic-scale studies of lithium diffusion, surfaces and voltage trends. <i>Journal of Materials Chemistry A</i> , 2014, 2, 7446-7453.	10.3	57
76	Layered $\text{LaSrGa}_3\text{O}_7$ -Based Oxide Ion Conductors: Cooperative Transport Mechanisms and Flexible Structures. <i>Advanced Functional Materials</i> , 2010, 20, 3874-3880.	14.9	56
77	Structure-Electronic Property Relationships of 2D Ruddlesden-Popper Tin- and Lead-based Iodide Perovskites. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 15328-15337.	8.0	56
78	Azetidinium lead iodide for perovskite solar cells. <i>Journal of Materials Chemistry A</i> , 2017, 5, 20658-20665.	10.3	53
79	Understanding the Enhanced Stability of Bromide Substitution in Lead Iodide Perovskites. <i>Chemistry of Materials</i> , 2020, 32, 400-409.	6.7	53
80	Insights into the increased degradation rate of $\text{CH}_3\text{NH}_3\text{PbI}_3$ solar cells in combined water and O_2 environments. <i>Journal of Materials Chemistry A</i> , 2017, 5, 25469-25475.	10.3	52
81	Vacancy and interstitial oxide ion migration in heavily doped $\text{La}_{2-x}\text{Sr}_x\text{CoO}_4$. <i>Journal of Materials Chemistry</i> , 2012, 22, 8969.	6.7	51
82	MgFeSiO_4 as a potential cathode material for magnesium batteries: ion diffusion rates and voltage trends. <i>Journal of Materials Chemistry A</i> , 2017, 5, 13161-13167.	10.3	51
83	A New Superionic Plastic Polymorph of the Na_3PS_4 Conductor. <i>Journal of Materials Chemistry A</i> , 2019, 1, 641-646.		50
84	Mechanochemical synthesis and ion transport properties of Na_3OX (X = Cl, Br, I and BH_4) antiperovskite solid electrolytes. <i>Journal of Power Sources</i> , 2020, 471, 228489.	7.8	47
85	Mixed ionic/electronic conductors $\text{Sr}_2\text{Fe}_2\text{O}_5$ and $\text{Sr}_4\text{Fe}_6\text{O}_{13}$: atomic-scale studies of defects and ion migration. <i>Journal of Materials Chemistry</i> , 2005, 15, 3200.	6.7	46
86	Structure of the nanocrystals in oxyfluoride glass ceramics. <i>Applied Physics Letters</i> , 2003, 83, 467-469.	3.3	42
87	Protonic defects and water incorporation in Si and Ge-based apatite ionic conductors. <i>Journal of Materials Chemistry</i> , 2010, 20, 2766.	6.7	36
88	A Combined Total Scattering and Simulation Approach to Analyzing Defect Structure in Bi_3YO_6 . <i>Chemistry of Materials</i> , 2010, 22, 4435-4445.	6.7	36
89	Computational Study of NaVOPO_4 Polymorphs as Cathode Materials for Na-Ion Batteries: Diffusion, Electronic Properties, and Cation-Doping Behavior. <i>Journal of Physical Chemistry C</i> , 2018, 122, 25829-25836.	3.1	36
90	Recent atomistic modelling studies of energy materials: batteries included. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2010, 368, 3255-3267.	3.4	35

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91	Strategies for the Optimisation of the Oxide Ion Conductivities of Apatite-type Germanates. Fuel Cells, 2011, 11, 10-16.	2.4	32
92	Evidence of Enhanced Ion Transport in Li-Rich Silicate Intercalation Materials. Advanced Energy Materials, 2017, 7, 1601043.	19.5	32
93	Structural and defect properties of the LaPO ₄ and La ₅ O ₁₄ -based proton conductors. Journal of Materials Chemistry, 2012, 22, 25388.	6.7	31
94	Alkali ion migration in albite and K-feldspar. Physics and Chemistry of Minerals, 2004, 31, 313-320.	0.8	30
95	Impact of Oxygen on the Electronic Structure of Triple-Cation Halide Perovskites. , 2019, 1, 506-510.		30
96	Lithium Migration Pathways and van der Waals Effects in the LiFeSO ₄ OH Battery Material. Chemistry of Materials, 2014, 26, 3672-3678.	6.7	26
97	Effect of Ba and Bi doping on the synthesis and sintering of Ge-based apatite phases. Journal of Solid State Electrochemistry, 2004, 8, 668.	2.5	25
98	Surfaces of Rutile MnO ₂ Are Electronically Conducting, Whereas the Bulk Material Is Insulating. Journal of Physical Chemistry C, 2014, 118, 25009-25015.	3.1	25
99	Deducing transport properties of mobile vacancies from perovskite solar cell characteristics. Journal of Applied Physics, 2020, 128, .	2.5	25
100	Tuning Ionic and Electronic Conductivities in the "Hollow" Perovskite {i>en}MAPbI ₃ . Chemistry of Materials, 2021, 33, 719-726.	6.7	24
101	Atomistic Insights into the Effects of Doping and Vacancy Clustering on Li-Ion Conduction in the Li ₃ OCl Antiperovskite Solid Electrolyte. ACS Applied Energy Materials, 2021, 4, 5094-5100.	5.1	24
102	Hop, skip or jump? Proton transport in the CaZrO ₃ perovskite oxide. Chemical Communications, 2001, , 661-662.	4.1	23
103	Insights into the Rich Polymorphism of the Na ⁺ Ion Conductor Na ₃ PS ₄ from the Perspective of Variable-Temperature Diffraction and Spectroscopy. Chemistry of Materials, 2021, 33, 5652-5667.	6.7	23
104	A Nanoscale Design Approach for Enhancing the Li-Ion Conductivity of the Li ₁₀ GeP ₂ S ₁₂ Solid Electrolyte. , 2022, 4, 424-431.		23
105	Atomic-scale investigation of cation doping and defect clustering in the anti-perovskite Na ₃ OCl sodium-ion conductor. Journal of Materials Chemistry A, 2022, 10, 2249-2255.	10.3	21
106	Surface phonons of lithium ion battery active materials. Sustainable Energy and Fuels, 2019, 3, 508-513.	4.9	18
107	Entropy Stabilization Effects and Ion Migration in 3D "Hollow" Halide Perovskites. Journal of the American Chemical Society, 2022, 144, 8223-8230.	13.7	18
108	Atomic Level Investigations of Lithium Ion Battery Cathode Materials. Journal of the Physical Society of Japan, 2010, 79, 59-64.	1.6	17

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109	Preparation of high-oxygen-content apatite silicates through Ti-doping: effect of Ti-doping on the oxide ion conductivity. <i>Journal of Materials Chemistry</i> , 2009, 19, 5003.	6.7	16
110	From Atoms to Cells: Multiscale Modeling of $\text{LiNi}_x\text{Mn}_y\text{Co}_z\text{O}_2$ Cathodes for Li-ion Batteries. <i>ACS Energy Letters</i> , 2022, 7, 108-122.	17.4	16
111	Novel Aspects of the Conduction Mechanisms of Electrolytes Containing Tetrahedral Moieties. <i>Fuel Cells</i> , 2011, 11, 38-43.	2.4	15
112	Quantifying the impact of disorder on Li-ion and Na-ion transport in perovskite titanate solid electrolytes for solid-state batteries. <i>Journal of Materials Chemistry A</i> , 2020, 8, 19603-19611.	10.3	15
113	Defect and dopant properties of the oxyfluoride superconductor $\text{Sr}_2\text{CuO}_2\text{F}_2$. <i>Physical Review B</i> , 1997, 55, 3141-3145.	3.2	14
114	Structural, Electronic, and Transport Properties of Hybrid SrTiO_3 -Graphene and Carbon Nanoribbon Interfaces. <i>Chemistry of Materials</i> , 2017, 29, 7364-7370.	6.7	14
115	Combined experimental and modelling studies of proton conducting $\text{La}_{1-x}\text{Ba}_{1+x}\text{GaO}_4$: proton location and dopant site selectivity. <i>Journal of Materials Chemistry</i> , 2010, 20, 10412.	6.7	12
116	Defect and dopant properties of the $\hat{1}\pm$ - and $\hat{1}^2$ -polymorphs of the Li_3FeF_6 lithium battery material. <i>Journal of Materials Chemistry A</i> , 2013, 1, 6588.	10.3	12
117	Ion migration in nepheline: a dielectric spectroscopy and computer modelling study. <i>Physics and Chemistry of Minerals</i> , 2001, 28, 28-34.	0.8	10
118	Defects in the new oxide-fluoride $\text{Ba}_2\text{PdO}_2\text{F}_2$: the search for fluoride needles in an oxide haystack. <i>Journal of Materials Chemistry</i> , 2005, 15, 119.	6.7	10
119	Lattice strain effects on doping, hydration and proton transport in scheelite-type electrolytes for solid oxide fuel cells. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 29330-29336.	2.8	9
120	COMPUTER SIMULATION STUDIES OF CERIA-BASED OXIDES. <i>Catalytic Science Series</i> , 2002, , 281-309.	0.0	7
121	Computer simulation of ion transport and hole centres in matlockite (PbFCl) structured phosphors. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , 1991, 64, 1119-1128.	0.6	6
122	Structural, Electronic, and Optical Properties of the Vacancy-Ordered Bismuth-Antimony Perovskites $(\text{CH}_3\text{NH}_3)_3(\text{Bi}_{1-x}\text{Sbx})_2\text{I}_9$. <i>Journal of Physical Chemistry C</i> , 2021, 125, 8938-8946.	3.1	5
123	Simulation studies of lithium intercalation in transition metal oxides. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , 1993, 68, 667-675.	0.6	4
124	Dopant Effects in the $\text{La}^{\text{III}}\text{O}_3$ Superconductor. <i>Molecular Simulation</i> , 1994, 12, 101-113.	2.0	4
125	Computer Modelling of Lithium and Proton Intercalation in Spinel Lithium Manganates: Effect of Octahedral Vacancies. <i>Molecular Crystals and Liquid Crystals</i> , 1998, 311, 109-114.	0.3	2
126	Energy Materials: Layered $\text{LaSrGa}_3\text{O}_7$ -Based Oxide-Ion Conductors: Cooperative Transport Mechanisms and Flexible Structures (<i>Adv. Funct. Mater.</i> 22/2010). <i>Advanced Functional Materials</i> , 2010, 20, 3809-3809.	14.9	1

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127	Energy materials for a low carbon future. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20190219.	3.4	1
128	Energy Spotlight. ACS Energy Letters, 2019, 4, 2763-2769.	17.4	1
129	An Ion Conducted Tour through LaMO ₃ Perovskite-based Oxide Materials. Molecular Simulation, 1998, 21, 127-141.	2.0	0
130	Oxygen Ion and Proton Transport in Mixed Metal Oxides. Materials Research Society Symposia Proceedings, 1998, 527, 457.	0.1	0
131	EXAFS studies of ceramic proton conductors. Radiation Effects and Defects in Solids, 2001, 155, 421-424.	1.2	0
132	The Synthesis and Characterisation of Ge Containing Apatite-Type Oxide Ion Conductors. Materials Research Society Symposia Proceedings, 2002, 756, 1.	0.1	0
133	Atomistic Exploration of the Surface-Sensitive Oriented Attachment Growth of a-MnCh Nanowires and the Formation of Defective Interface with 2Å–3 and 2Å–4 Tunnel Intergrowth. Microscopy and Microanalysis, 2016, 22, 386-387.	0.4	0
134	The Degradation Mechanism of Tin Perovskite Solar Cells and the Critical Role of Tin (IV) Iodide. , 0, , .		0
135	From MAPI to Mixed A-Cation Perovskites: Atomic-Scale Insights into Defects, Diffusion & Dynamics. , 0, , .		0
136	Structural Distortion and Molecular Cation Dynamics in Mixed-Cation Perovskites. , 0, , .		0
137	Optical and Electronic Property Changes in Lead-free Perovskites by Metal Cation Transmutation. , 0, , .		0
138	Atomic-Scale Insights into Lead and Tin Perovskite Materials: Ion Transport, Cation Substitution & Degradation Mechanisms. , 0, , .		0
139	Degradation Mechanism of Hybrid Tin Perovskite and the Critical Role of Tin (IV) Iodide. , 0, , .		0