

M Saiful Islam

List of Publications by Year in descending order

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139
papers

17,951
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13827

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docs citations

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times ranked

18275
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#	ARTICLE	IF	CITATIONS
1	Atomic-scale investigation of cation doping and defect clustering in the anti-perovskite Na ₃ OCl sodium-ion conductor. <i>Journal of Materials Chemistry A</i> , 2022, 10, 2249-2255.	5.2	21
2	From Atoms to Cells: Multiscale Modeling of LiNi _x Mn _y Co _z O ₂ Cathodes for Li-Ion Batteries. <i>ACS Energy Letters</i> , 2022, 7, 108-122.	8.8	16
3	A Nanoscale Design Approach for Enhancing the Li-Ion Conductivity of the Li ₁₀ GeP ₂ S ₁₂ Solid Electrolyte. <i>Journal of Materials Chemistry A</i> , 2022, 4, 424-431.		23
4	Entropy Stabilization Effects and Ion Migration in 3D "Hollow" Halide Perovskites. <i>Journal of the American Chemical Society</i> , 2022, 144, 8223-8230.	6.6	18
5	Tuning Ionic and Electronic Conductivities in the "Hollow" Perovskite {MAPbI ₃ }. <i>Chemistry of Materials</i> , 2021, 33, 719-726.	3.2	24
6	Atomistic Insights into the Effects of Doping and Vacancy Clustering on Li-Ion Conduction in the Li ₃ OCl Antiperovskite Solid Electrolyte. <i>ACS Applied Energy Materials</i> , 2021, 4, 5094-5100.	2.5	24
7	Structural, Electronic, and Optical Properties of the Vacancy-Ordered Bismuth-Antimony Perovskites (CH ₃ NH ₃) ₃ (Bi _{1-x} Sb _x) ₂ I ₉ . <i>Journal of Physical Chemistry C</i> , 2021, 125, 8938-8946.	1.5	5
8	Degradation mechanism of hybrid tin-based perovskite solar cells and the critical role of tin (IV) iodide. <i>Nature Communications</i> , 2021, 12, 2853.	5.8	236
9	Insights into the Rich Polymorphism of the Na ⁺ Ion Conductor Na ₃ PS ₄ from the Perspective of Variable-Temperature Diffraction and Spectroscopy. <i>Chemistry of Materials</i> , 2021, 33, 5652-5667.	3.2	23
10	Understanding the Enhanced Stability of Bromide Substitution in Lead Iodide Perovskites. <i>Chemistry of Materials</i> , 2020, 32, 400-409.	3.2	53
11	Under Pressure: Mechanochemical Effects on Structure and Ion Conduction in the Sodium-Ion Solid Electrolyte Na ₃ PS ₄ . <i>Journal of the American Chemical Society</i> , 2020, 142, 18422-18436.	6.6	58
12	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.	5.2	15
13	Redox Chemistry and the Role of Trapped Molecular O ₂ in Li-Rich Disordered Rocksalt Oxyfluoride Cathodes. <i>Journal of the American Chemical Society</i> , 2020, 142, 21799-21809.	6.6	77
14	Deducing transport properties of mobile vacancies from perovskite solar cell characteristics. <i>Journal of Applied Physics</i> , 2020, 128, .	1.1	25
15	Structure-Electronic Property Relationships of 2D Ruddlesden-Popper Tin- and Lead-based Iodide Perovskites. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 15328-15337.	4.0	56
16	Mechanochemical synthesis and ion transport properties of Na ₃ OX (X = Cl, Br, I and BH ₄) antiperovskite solid electrolytes. <i>Journal of Power Sources</i> , 2020, 471, 228489.	4.0	47
17	Fundamentals of inorganic solid-state electrolytes for batteries. <i>Nature Materials</i> , 2019, 18, 1278-1291.	13.3	1,341
18	Energy materials for a low carbon future. <i>Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences</i> , 2019, 377, 20190219.	1.6	1

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19	Toward Understanding the Different Influences of Grain Boundaries on Ion Transport in Sulfide and Oxide Solid Electrolytes. <i>Chemistry of Materials</i> , 2019, 31, 5296-5304.	3.2	89
20	A New Superionic Plastic Polymorph of the Na ⁺ Conductor Na ₃ PS ₄ . , 2019, 1, 641-646.		50
21	Energy Spotlight. <i>ACS Energy Letters</i> , 2019, 4, 2763-2769.	8.8	1
22	Impact of Oxygen on the Electronic Structure of Triple-Cation Halide Perovskites. , 2019, 1, 506-510.		30
23	Surface phonons of lithium ion battery active materials. <i>Sustainable Energy and Fuels</i> , 2019, 3, 508-513.	2.5	18
24	Putting the Squeeze on Lead Iodide Perovskites: Pressure-Induced Effects To Tune Their Structural and Optoelectronic Behavior. <i>Chemistry of Materials</i> , 2019, 31, 4063-4071.	3.2	87
25	Partial cation substitution reduces iodide ion transport in lead iodide perovskite solar cells. <i>Energy and Environmental Science</i> , 2019, 12, 2264-2272.	15.6	168
26	Depth-dependent oxygen redox activity in lithium-rich layered oxide cathodes. <i>Journal of Materials Chemistry A</i> , 2019, 7, 25355-25368.	5.2	62
27	The Impact of Atmosphere on the Local Luminescence Properties of Metal Halide Perovskite Grains. <i>Advanced Materials</i> , 2018, 30, e1706208.	11.1	149
28	Lead-Free Perovskite Semiconductors Based on Germanium–Tin Solid Solutions: Structural and Optoelectronic Properties. <i>Journal of Physical Chemistry C</i> , 2018, 122, 5940-5947.	1.5	104
29	Particle Morphology and Lithium Segregation to Surfaces of the Li ₇ La ₃ Zr ₂ O ₁₂ Solid Electrolyte. <i>Chemistry of Materials</i> , 2018, 30, 3019-3027.	3.2	80
30	Crystal Structures, Local Atomic Environments, and Ion Diffusion Mechanisms of Scandium-Substituted Sodium Superionic Conductor (NASICON) Solid Electrolytes. <i>Chemistry of Materials</i> , 2018, 30, 2618-2630.	3.2	109
31	High voltage structural evolution and enhanced Na-ion diffusion in P ₂ -Na _{2/3} Ni _{1/3} Mg _x Mn _{2/3} O ₂ (0 x <math>< i>Tj ETQq1 1 0.7843</math>). <i>Environmental Science</i> . 2018. 11. 1470-1479.	15.6	148
32	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.	6.6	226
33	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.	1.5	36
34	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.	1.5	59
35	A review of structural properties and synthesis methods of solid electrolyte materials in the Li ₂ S–P ₂ S ₅ binary system. <i>Journal of Power Sources</i> , 2018, 407, 31-43.	4.0	140
36	Fluid-enhanced surface diffusion controls intraparticle phase transformations. <i>Nature Materials</i> , 2018, 17, 915-922.	13.3	104

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37	Phase Behavior and Polymorphism of Formamidinium Lead Iodide. <i>Chemistry of Materials</i> , 2018, 30, 3768-3778.	3.2	104
38	Elucidating lithium-ion and proton dynamics in anti-perovskite solid electrolytes. <i>Energy and Environmental Science</i> , 2018, 11, 2993-3002.	15.6	95
39	Mixed A-Cation Perovskites for Solar Cells: Atomic-Scale Insights Into Structural Distortion, Hydrogen Bonding, and Electronic Properties. <i>Chemistry of Materials</i> , 2018, 30, 5194-5204.	3.2	127
40	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.	4.0	147
41	Evidence of Enhanced Ion Transport in Li-Rich Silicate Intercalation Materials. <i>Advanced Energy Materials</i> , 2017, 7, 1601043.	10.2	32
42	Fast oxygen diffusion and iodide defects mediate oxygen-induced degradation of perovskite solar cells. <i>Nature Communications</i> , 2017, 8, 15218.	5.8	917
43	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.	5.2	51
44	Understanding the stability of mixed A-cation lead iodide perovskites. <i>Journal of Materials Chemistry A</i> , 2017, 5, 22495-22499.	5.2	91
45	Good Vibrations: Locking of Octahedral Tilting in Mixed-Cation Iodide Perovskites for Solar Cells. <i>ACS Energy Letters</i> , 2017, 2, 2424-2429.	8.8	126
46	Azetidinium lead iodide for perovskite solar cells. <i>Journal of Materials Chemistry A</i> , 2017, 5, 20658-20665.	5.2	53
47	Structural, Electronic, and Transport Properties of Hybrid SrTiO ₃ -Graphene and Carbon Nanoribbon Interfaces. <i>Chemistry of Materials</i> , 2017, 29, 7364-7370.	3.2	14
48	Insights into the increased degradation rate of CH ₃ NH ₃ PbI ₃ solar cells in combined water and O ₂ environments. <i>Journal of Materials Chemistry A</i> , 2017, 5, 25469-25475.	5.2	52
49	Mechanisms of Lithium Intercalation and Conversion Processes in Organic-Inorganic Halide Perovskites. <i>ACS Energy Letters</i> , 2017, 2, 1818-1824.	8.8	111
50	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. <i>Microscopy and Microanalysis</i> , 2016, 22, 386-387.	0.2	0
51	Lithium Extraction Mechanism in Li-Rich Li ₂ MnO ₃ Involving Oxygen Hole Formation and Dimerization. <i>Chemistry of Materials</i> , 2016, 28, 6656-6663.	3.2	210
52	The influence of large cations on the electrochemical properties of tunnel-structured metal oxides. <i>Nature Communications</i> , 2016, 7, 13374.	5.8	180
53	Na ₂ CoSiO ₄ as a cathode material for sodium-ion batteries: structure, electrochemistry and diffusion pathways. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 32744-32752.	1.3	69
54	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.	1.3	9

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55	Feeling the strain: enhancing ionic transport in olivine phosphate cathodes for Li- and Na-ion batteries through strain effects. <i>Journal of Materials Chemistry A</i> , 2016, 4, 6998-7004.	5.2	59
56	Atomistic Insights into the Oriented Attachment of Tunnel-Based Oxide Nanostructures. <i>ACS Nano</i> , 2016, 10, 539-548.	7.3	66
57	Structural and Mechanistic Insights into Fast Lithium-Ion Conduction in Li_4SiO_4 "Li ₃ PO ₄ Solid Electrolytes. <i>Journal of the American Chemical Society</i> , 2015, 137, 9136-9145.	6.6	223
58	Ionic transport in hybrid lead iodide perovskite solar cells. <i>Nature Communications</i> , 2015, 6, 7497.	5.8	2,154
59	Sodium Ion Diffusion and Voltage Trends in Phosphates $\text{Na}_4\text{M}_3(\text{PO}_4)_2\text{P}_2\text{O}_7$ (M = Fe,) <i>Tj ETQ</i> 1 0.784014 rgBT	11.1	140
60	Surfaces of Rutile MnO_2 Are Electronically Conducting, Whereas the Bulk Material Is Insulating. <i>Journal of Physical Chemistry C</i> , 2014, 118, 25009-25015.	1.5	25
61	Lithium and sodium battery cathode materials: computational insights into voltage, diffusion and nanostructural properties. <i>Chemical Society Reviews</i> , 2014, 43, 185-204.	18.7	899
62	Surface properties of $\hat{\Gamma}$ - MnO_2 : relevance to catalytic and supercapacitor behaviour. <i>Journal of Materials Chemistry A</i> , 2014, 2, 15509-15518.	5.2	121
63	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.	5.2	57
64	Lithium Migration Pathways and van der Waals Effects in the LiFeSO_4OH Battery Material. <i>Chemistry of Materials</i> , 2014, 26, 3672-3678.	3.2	26
65	Rutile ($\hat{\Gamma}$ -) MnO_2 Surfaces and Vacancy Formation for High Electrochemical and Catalytic Performance. <i>Journal of the American Chemical Society</i> , 2014, 136, 1418-1426.	6.6	186
66	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. <i>Journal of Materials Chemistry A</i> , 2014, 2, 11807-11812.	5.2	92
67	Defect chemistry and lithium-ion migration in polymorphs of the cathode material $\text{Li}_2\text{MnSiO}_4$. <i>Journal of Materials Chemistry A</i> , 2013, 1, 4207.	5.2	113
68	Na-ion mobility in layered $\text{Na}_2\text{FePO}_4\text{F}$ and olivine $\text{Na}[\text{Fe},\text{Mn}]\text{PO}_4$. <i>Energy and Environmental Science</i> , 2013, 6, 2257.	15.6	228
69	Nanostructuring of $\hat{\Gamma}$ - MnO_2 : The Important Role of Surface to Bulk Ion Migration. <i>Chemistry of Materials</i> , 2013, 25, 536-541.	3.2	99
70	Defect and dopant properties of the $\hat{\Gamma}$ - and $\hat{\Gamma}$ -polymorphs of the Li_3FeF_6 lithium battery material. <i>Journal of Materials Chemistry A</i> , 2013, 1, 6588.	5.2	12
71	Electrochemistry of Hollandite $\hat{\Gamma}$ - MnO_2 : Li-Ion and Na-Ion Insertion and Li_2O Incorporation. <i>Chemistry of Materials</i> , 2013, 25, 2515-2526.	3.2	172
72	Complete structural model for lanthanum tungstate: a chemically stable high temperature proton conductor by means of intrinsic defects. <i>Journal of Materials Chemistry</i> , 2012, 22, 1762-1764.	6.7	91

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73	Insights into Changes in Voltage and Structure of $\text{Li}_{2-x}\text{FeSiO}_4$ Polymorphs for Lithium-Ion Batteries. <i>Chemistry of Materials</i> , 2012, 24, 2155-2161.	3.2	128
74	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
75	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.	1.5	204
76	Structural and defect properties of the LaPO_4 and La_5O_{14} -based proton conductors. <i>Journal of Materials Chemistry</i> , 2012, 22, 25388.	6.7	31
77	Structure and Lithium Transport Pathways in $\text{Li}_{2-x}\text{FeSiO}_4$ Cathodes for Lithium Batteries. <i>Journal of the American Chemical Society</i> , 2011, 133, 13031-13035.	6.6	277
78	Alkali-ion Conduction Paths in LiFeSO_4F and NaFeSO_4F Layer-Type Cathode Materials. <i>Chemistry of Materials</i> , 2011, 23, 2278-2284.	3.2	156
79	The lithium intercalation process in the low-voltage lithium battery anode $\text{Li}_{1+x}\text{V}_2\text{O}_7$. <i>Nature Materials</i> , 2011, 10, 223-229.	13.3	267
80	Silicate cathodes for lithium batteries: alternatives to phosphates?. <i>Journal of Materials Chemistry</i> , 2011, 21, 9811.	6.7	310
81	Strategies for the Optimisation of the Oxide Ion Conductivities of Apatite-Type Germanates. <i>Fuel Cells</i> , 2011, 11, 10-16.	1.5	32
82	Novel Aspects of the Conduction Mechanisms of Electrolytes Containing Tetrahedral Moieties. <i>Fuel Cells</i> , 2011, 11, 38-43.	1.5	15
83	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
84	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.	7.8	56
85	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.	7.8	1
86	Defect chemistry and proton-dopant association in BaZrO_3 and BaPrO_3 . <i>Journal of Materials Chemistry</i> , 2010, 20, 6258.	6.7	145
87	Atomic Level Investigations of Lithium Ion Battery Cathode Materials. <i>Journal of the Physical Society of Japan</i> , 2010, 79, 59-64.	0.7	17
88	Anti-Site Defects and Ion Migration in the $\text{Li}_{0.5}\text{Mn}_{0.5}\text{PO}_4$ Mixed-Metal Cathode Material. <i>Chemistry of Materials</i> , 2010, 22, 1242-1248.	3.2	140
89	A Combined Total Scattering and Simulation Approach to Analyzing Defect Structure in Bi_3YO_6 . <i>Chemistry of Materials</i> , 2010, 22, 4435-4445.	3.2	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.	1.6	35

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91	Defects, Dopants, and Protons in LaNbO_4 . Chemistry of Materials, 2010, 22, 5912-5917.	3.2	59
92	Lithium Coordination Sites in $\text{Li}_x\text{TiO}_2(\text{B})$: A Structural and Computational Study. Chemistry of Materials, 2010, 22, 6426-6432.	3.2	104
93	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. Journal of Materials Chemistry, 2010, 20, 10412.	6.7	12
94	$\text{Li}_2\text{MnSiO}_4$ Lithium Battery Material: Atomic-Scale Study of Defects, Lithium Mobility, and Trivalent Dopants. Chemistry of Materials, 2009, 21, 5196-5202.	3.2	160
95	Lithium Insertion and Transport in the TiO_2 -B Anode Material: A Computational Study. Chemistry of Materials, 2009, 21, 4778-4783.	3.2	169
96	Preparation of high-oxygen-content apatite silicates through Ti-doping: effect of Ti-doping on the oxide ion conductivity. Journal of Materials Chemistry, 2009, 19, 5003.	6.7	16
97	Atomic-Scale Insight into LaFeO_3 Perovskite: Defect Nanoclusters and Ion Migration. Journal of Physical Chemistry C, 2008, 112, 4455-4462.	1.5	100
98	Surface structures and crystal morphologies of LiFePO_4 : relevance to electrochemical behaviour. Journal of Materials Chemistry, 2008, 18, 1209.	6.7	232
99	Lithium Battery Materials Li_xMPO_4 ($\text{M} = \text{Mn, Fe, Co, and Ni}$): Insights into Defect Association, Transport Mechanisms, and Doping Behavior. Chemistry of Materials, 2008, 20, 5907-5915.	3.2	483
100	Developing apatites for solid oxide fuel cells: insight into structural, transport and doping properties. Journal of Materials Chemistry, 2007, 17, 3104.	6.7	239
101	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.	1.2	72
102	Atomic-Scale Investigation of Defects, Dopants, and Lithium Transport in the LiFePO_4 Olivine-Type Battery Material. Chemistry of Materials, 2005, 17, 5085-5092.	3.2	966
103	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. Journal of Materials Chemistry, 2005, 15, 3200.	6.7	46
104	Defects in the new oxide-fluoride $\text{Ba}_2\text{PdO}_2\text{F}_2$: the search for fluoride needles in an oxide haystack. Journal of Materials Chemistry, 2005, 15, 119.	6.7	10
105	Effect of Ba and Bi doping on the synthesis and sintering of Ge-based apatite phases. Journal of Solid State Electrochemistry, 2004, 8, 668.	1.2	25
106	Alkali ion migration in albite and K-feldspar. Physics and Chemistry of Minerals, 2004, 31, 313-320.	0.3	30
107	Doping and defect association in AZrO_3 ($\text{A} = \text{Ca, Ba}$) and LaMO_3 ($\text{M} = \text{Sc, Ga}$) perovskite-type ionic conductors. Dalton Transactions, 2004, , 3061.	1.6	106
108	Atomistic study of dopant site-selectivity and defect association in the lanthanum gallate perovskite. Journal of Materials Chemistry, 2004, 14, 86.	6.7	96

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109	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 . Journal of Materials Chemistry, 2003, 13, 1956.	6.7	250
110	Reduction Process in CeO ₂ ~MO and CeO ₂ ~M ₂ O ₃ Mixed Oxides: A Computer Simulation Study. Chemistry of Materials, 2003, 15, 3781-3785.	3.2	82
111	Structure of the nanocrystals in oxyfluoride glass ceramics. Applied Physics Letters, 2003, 83, 467-469.	1.5	42
112	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.	2.2	127
113	The Synthesis and Characterisation of Ge Containing Apatite-Type Oxide Ion Conductors. Materials Research Society Symposia Proceedings, 2002, 756, 1.	0.1	0
114	COMPUTER SIMULATION STUDIES OF CERIA-BASED OXIDES. Catalytic Science Series, 2002, , 281-309.	0.6	7
115	Hop, skip or jump? Proton transport in the CaZrO ₃ perovskite oxide. Chemical Communications, 2001, , 661-662.	2.2	23
116	Proton Migration and Defect Interactions in the CaZrO ₃ Orthorhombic Perovskite: A Quantum Mechanical Study. Chemistry of Materials, 2001, 13, 2049-2055.	3.2	142
117	Surface structures and defect properties of pure and doped La ₂ NiO ₄ . Journal of Materials Chemistry, 2001, 11, 2597-2602.	6.7	75
118	EXAFS studies of ceramic proton conductors. Radiation Effects and Defects in Solids, 2001, 155, 421-424.	0.4	0
119	Ion migration in nepheline: a dielectric spectroscopy and computer modelling study. Physics and Chemistry of Minerals, 2001, 28, 28-34.	0.3	10
120	Defect chemistry and surface properties of LaCoO ₃ . Journal of Materials Chemistry, 2000, 10, 2298-2305.	6.7	107
121	Bulk Reduction and Oxygen Migration in the Ceria-Based Oxides. Chemistry of Materials, 2000, 12, 677-681.	3.2	157
122	Ionic transport in ABO ₃ perovskite oxides: a computer modelling tour. Journal of Materials Chemistry, 2000, 10, 1027-1038.	6.7	453
123	Computer Modelling of Lithium and Proton Intercalation in Spinel Lithium Manganates: Effect of Octahedral Vacancies. Molecular Crystals and Liquid Crystals, 1998, 311, 109-114.	0.3	2
124	An Ion Conducted Tour through LaMO ₃ Perovskite-based Oxide Materials. Molecular Simulation, 1998, 21, 127-141.	0.9	0
125	Surface and Reduction Energetics of the CeO ₂ ~ZrO ₂ Catalysts. Journal of Physical Chemistry B, 1998, 102, 557-561.	1.2	208
126	Dopant Substitution and Ion Migration in the LaGaO ₃ -Based Oxygen Ion Conductor. Journal of Physical Chemistry B, 1998, 102, 3099-3104.	1.2	142

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127	Oxygen Ion and Proton Transport in Mixed Metal Oxides. Materials Research Society Symposia Proceedings, 1998, 527, 457.	0.1	0
128	Defect and dopant properties of the oxyfluoride superconductor Sr ₂ CuO ₂ F ₂ + δ s. Physical Review B, 1997, 55, 3141-3145.	1.1	14
129	Atomistic Simulation Studies of Lithium and Proton Insertion in Spinel Lithium Manganates. Journal of Physical Chemistry B, 1997, 101, 8156-8163.	1.2	98
130	Computer Simulation Studies of Bulk Reduction and Oxygen Migration in CeO ₂ -ZrO ₂ Solid Solutions. Journal of Physical Chemistry B, 1997, 101, 1750-1753.	1.2	240
131	Dopant Effects in the δ -Bi ₂ Superconductor. Molecular Simulation, 1994, 12, 101-113.	0.9	4
132	Simulation studies of lithium intercalation in transition metal oxides. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1993, 68, 667-675.	0.8	4
133	Computer simulation of ion transport and hole centres in mallockite (PbFCl) structured phosphors. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1991, 64, 1119-1128.	0.8	6
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