

Rotraut Merkle

List of Publications by Year in descending order

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51
papers

2,978
citations

201674

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51
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51
all docs

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docs citations

51
times ranked

3205
citing authors

#	ARTICLE	IF	CITATIONS
1	How Is Oxygen Incorporated into Oxides? A Comprehensive Kinetic Study of a Simple Solid-State Reaction with SrTiO ₃ as a Model Material. <i>Angewandte Chemie - International Edition</i> , 2008, 47, 3874-3894.	13.8	325
2	Combined theoretical and experimental analysis of processes determining cathode performance in solid oxide fuel cells. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 5443.	2.8	240
3	Mixed-Conducting Perovskites as Cathode Materials for Protonic Ceramic Fuel Cells: Understanding the Trends in Proton Uptake. <i>Advanced Functional Materials</i> , 2018, 28, 1801241.	14.9	198
4	Pathways for Oxygen Incorporation in Mixed Conducting Perovskites: A DFT-Based Mechanistic Analysis for (La, Sr)MnO ₃ . <i>Journal of Physical Chemistry C</i> , 2010, 114, 3017-3027.	3.1	160
5	Interaction of oxygen with halide perovskites. <i>Journal of Materials Chemistry A</i> , 2018, 6, 10847-10855.	10.3	140
6	Jahn-Teller distortion around Fe^{4+} in FeMnO_4 . <i>Journal of Materials Chemistry A</i> , 2018, 6, 10847-10855.		

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19	Stoichiometry Variation in Materials with Three Mobile Carriers—Thermodynamics and Transport Kinetics Exemplified for Protons, Oxygen Vacancies, and Holes. <i>Advanced Functional Materials</i> , 2015, 25, 1542-1557.	14.9	64
20	Oxides with Mixed Protonic and Electronic Conductivity. <i>Annual Review of Materials Research</i> , 2021, 51, 461-493.	9.3	49
21	Optically Tuning the Rate of Stoichiometry Changes: Surface-Controlled Oxygen Incorporation into Oxides under UV Irradiation. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 2126-2129.	13.8	48
22	Slow CH_3NH_3^+ Diffusion in $\text{CH}_3\text{NH}_3\text{PbI}_3$ under Light Measured by Solid-State NMR and Tracer Diffusion. <i>Journal of Physical Chemistry C</i> , 2018, 122, 21803-21806.	3.1	46
23	The significance of defect chemistry for the rate of gas-solid reactions: three examples. <i>Topics in Catalysis</i> , 2006, 38, 141-145.	2.8	38
24	Surface termination effects on the oxygen reduction reaction rate at fuel cell cathodes. <i>Journal of Materials Chemistry A</i> , 2018, 6, 11929-11940.	10.3	38
25	Ab initio modelling of oxygen vacancies and protonic defects in $\text{La}_{1-x}\text{Sr}_x\text{FeO}_{3-\delta}$ perovskite solid solutions. <i>Journal of Materials Chemistry A</i> , 2016, 4, 13093-13104.	10.3	33
26	Oxygen exchange kinetics on systematically doped ceria: a pulsed isotope exchange study. <i>Journal of Materials Chemistry A</i> , 2019, 7, 21854-21866.	10.3	32
27	Oxygen Reduction at Dense Thin-Film Microelectrodes on a Proton-Conducting Electrolyte. <i>Journal of the Electrochemical Society</i> , 2015, 162, F939-F950.	2.9	29
28	Humidity-Controlled Water Uptake and Conductivities in Ion and Electron Mixed Conducting Polythiophene Films. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 6742-6751.	8.0	29
29	Effects of NiO addition on sintering and proton uptake of $\text{Ba}(\text{Zr,Ce,Y})\text{O}_{3-\delta}$. <i>Journal of Materials Chemistry A</i> , 2021, 9, 14775-14785.	10.3	27
30	Investigation of oxygen exchange kinetics in proton-conducting ceramic fuel cells: Effect of electronic leakage current using symmetric cells. <i>Journal of Power Sources</i> , 2013, 242, 784-789.	7.8	24
31	Interdependence of Oxygenation and Hydration in Mixed-Conducting $(\text{Ba,Sr})\text{FeO}_{3-\delta}$ Perovskites Studied by Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2020, 124, 11780-11789.	3.1	24
32	Proton, Hydroxide Ion, and Oxide Ion Affinities of Closed-Shell Oxides: Importance for the Hydration Reaction and Correlation to Electronic Structure. <i>Journal of Physical Chemistry C</i> , 2020, 124, 1277-1284.	3.1	23
33	First principles calculations of oxygen reduction reaction at fuel cell cathodes. <i>Current Opinion in Electrochemistry</i> , 2020, 19, 122-128.	4.8	23
34	X-ray Spectroscopy of $(\text{Ba,Sr,La})(\text{Fe,Zn,Y})\text{O}_{3-\delta}$ Identifies Structural and Electronic Features Favoring Proton Uptake. <i>Chemistry of Materials</i> , 2020, 32, 8502-8511.	6.7	23
35	Effect of NiO addition on proton uptake of $\text{BaZr}_{1-x}\text{Y}_x\text{O}_{3-x/2}$ and $\text{BaZr}_{1-x}\text{Sc}_x\text{O}_{3-x/2}$ electrolytes. <i>Solid State Ionics</i> , 2020, 347, 115256.	2.7	22
36	Mixed conductivity of polythiophene-based ionic polymers under controlled conditions. <i>Polymer</i> , 2017, 132, 216-226.	3.8	21

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37	Impact of point defects on the elastic properties of BaZrO ₃ : Comprehensive insight from experiments and ab initio calculations. Acta Materialia, 2018, 160, 247-256.	7.9	21
38	Bulk Defect Chemistry of PCFC Cathode Materials: Discussion of Defect Interactions. ECS Transactions, 2017, 77, 133-138.	0.5	15
39	PLD-deposited (Ba _x Sr _{1-x})(Co _y Fe _{1-y})O _{3-δ} Thin-Film Microelectrodes: Structure Aspects and Oxygen Incorporation Kinetics. ECS Transactions, 2008, 13, 85-95.	0.5	14
40	(Invited) Oxygen Reduction Reaction at Cathodes on Proton Conducting Oxide Electrolytes: Contribution from Three Phase Boundary Compared to Bulk Path. ECS Transactions, 2015, 66, 95-102.	0.5	14
41	Influence of Y-substitution on phase composition and proton uptake of self-generated Ba(Ce,Fe)O _{3-δ} Ba(Fe,Ce)O _{3-δ} composites. Journal of Materials Chemistry A, 2022, 10, 2474-2482.	10.3	13
42	Influence of hydration and dopant ionic radius on the elastic properties of BaZrO ₃ . Solid State Ionics, 2020, 344, 115130.	2.7	11
43	Probing Charge Accumulation at SrMnO ₃ /SrTiO ₃ Heterointerfaces via Advanced Electron Microscopy and Spectroscopy. ACS Nano, 2020, 14, 12697-12707.	14.6	9
44	Defect chemistry and proton uptake of La _{2-x} Sr _x NiO _{4-δ} and La _{2-x} Ba _x NiO _{4-δ} Ruddlesden-Popper phases. Journal of Solid State Chemistry, 2022, 306, 122731.	2.9	9
45	Synthesis, characterization and thermal behaviour of solid phases in the quasi-ternary system Mg(SCN) ₂ ·H ₂ O·THF. Dalton Transactions, 2021, 50, 6949-6961.	3.3	8
46	Fabrication of multi-layered structures for proton conducting ceramic cells. Journal of Materials Chemistry A, 2022, 10, 2362-2373.	10.3	8
47	Non-Classical Electrostriction in Hydrated Acceptor Doped BaZrO ₃ : Proton Trapping and Dopant Size Effect. Advanced Functional Materials, 2021, 31, 2104188.	14.9	8
48	Electronic modifications in (Ba,La)(Fe,Zn,Y)O _{3-δ} unveiled by oxygen K-edge X-ray Raman scattering. Journal of Materials Chemistry A, 2022, 10, 8866-8876.	10.3	7
49	Interdependence of Point Defects and Reaction Kinetics: CO and CH ₄ Oxidation on Ceria and Zirconia. Journal of Physical Chemistry C, 2020, 124, 18544-18556.	3.1	5
50	On the crystal structures of lithium thiocyanate monohydrate LiSCN \cdot H ₂ O and the phase diagram LiSCN \cdot H ₂ O. Journal of Physics and Chemistry of Solids, 2022, 160, 110299.	4.0	4
51	(Invited) The Effect of (La,Sr)MnO ₃ Cathode Surface Termination on Its Electronic Structure. ECS Transactions, 2017, 77, 67-73.	0.5	2