

Rotraut Merkle

List of Publications by Year in descending order

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51
papers

2,978
citations

201674

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182427

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docs citations

51
times ranked

3205
citing authors

#	ARTICLE	IF	CITATIONS
1	Fabrication of multi-layered structures for proton conducting ceramic cells. Journal of Materials Chemistry A, 2022, 10, 2362-2373.	10.3	8
2	On the crystal structures of lithium thiocyanate monohydrate $\text{LiSCN} \cdot \text{H}_2\text{O}$ and the phase diagram $\text{LiSCN} - \text{H}_2\text{O}$. Journal of Physics and Chemistry of Solids, 2022, 160, 110299.	4.0	4
3	Defect chemistry and proton uptake of $\text{La}_{2-x}\text{Sr}_x\text{NiO}_{4\pm\delta}$ and $\text{La}_{2-x}\text{Ba}_x\text{NiO}_{4\pm\delta}$ Ruddlesden-Popper phases. Journal of Solid State Chemistry, 2022, 306, 122731.	2.9	9
4	Influence of Y-substitution on phase composition and proton uptake of self-generated $\text{Ba}(\text{Ce},\text{Fe})\text{O}_{3\delta}$ composites. Journal of Materials Chemistry A, 2022, 10, 2474-2482.	10.3	13
5	Electronic modifications in $(\text{Ba},\text{La})(\text{Fe},\text{Zn},\text{Y})\text{O}_{3\delta}$ unveiled by oxygen K-edge X-ray Raman scattering. Journal of Materials Chemistry A, 2022, 10, 8866-8876.	10.3	7
6	Synthesis, characterization and thermal behaviour of solid phases in the quasi-ternary system $\text{Mg}(\text{SCN})_2 - \text{H}_2\text{O} - \text{THF}$. Dalton Transactions, 2021, 50, 6949-6961.	3.3	8
7	Effects of NiO addition on sintering and proton uptake of $\text{Ba}(\text{Zr},\text{Ce},\text{Y})\text{O}_{3\delta}$. Journal of Materials Chemistry A, 2021, 9, 14775-14785.	10.3	27
8	Oxides with Mixed Protonic and Electronic Conductivity. Annual Review of Materials Research, 2021, 51, 461-493.	9.3	49
9	Non-Classical Electrostriction in Hydrated Acceptor Doped BaZrO_3 : Proton Trapping and Dopant Size Effect. Advanced Functional Materials, 2021, 31, 2104188.	14.9	8
10	Influence of hydration and dopant ionic radius on the elastic properties of BaZrO_3 . Solid State Ionics, 2020, 344, 115130.	2.7	11
11	Proton, Hydroxide Ion, and Oxide Ion Affinities of Closed-Shell Oxides: Importance for the Hydration Reaction and Correlation to Electronic Structure. Journal of Physical Chemistry C, 2020, 124, 1277-1284.	3.1	23
12	First principles calculations of oxygen reduction reaction at fuel cell cathodes. Current Opinion in Electrochemistry, 2020, 19, 122-128.	4.8	23
13	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
14	X-ray Spectroscopy of $(\text{Ba},\text{Sr},\text{La})(\text{Fe},\text{Zn},\text{Y})\text{O}_{3\delta}$ Identifies Structural and Electronic Features Favoring Proton Uptake. Chemistry of Materials, 2020, 32, 8502-8511.	6.7	23
15	Probing Charge Accumulation at $\text{SrMnO}_3/\text{SrTiO}_3$ Heterointerfaces via Advanced Electron Microscopy and Spectroscopy. ACS Nano, 2020, 14, 12697-12707.	14.6	9
16	Interdependence of Oxygenation and Hydration in Mixed-Conducting $(\text{Ba},\text{Sr})\text{FeO}_{3\delta}$ Perovskites Studied by Density Functional Theory. Journal of Physical Chemistry C, 2020, 124, 11780-11789.	3.1	24
17	Humidity-Controlled Water Uptake and Conductivities in Ion and Electron Mixed Conducting Polythiophene Films. ACS Applied Materials & Interfaces, 2020, 12, 6742-6751.	8.0	29
18	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. Solid State Ionics, 2020, 347, 115256.	2.7	22

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19	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
20	Impact of point defects on the elastic properties of BaZrO ₃ : Comprehensive insight from experiments and ab initio calculations. <i>Acta Materialia</i> , 2018, 160, 247-256.	7.9	21
21	Slow CH ₃ NH ₃ ⁺ Diffusion in CH ₃ NH ₃ 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
22	Interaction of oxygen with halide perovskites. <i>Journal of Materials Chemistry A</i> , 2018, 6, 10847-10855.	10.3	140
23	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
24	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
25	(Invited) The Effect of (La,Sr)MnO ₃ Cathode Surface Termination on Its Electronic Structure. <i>ECS Transactions</i> , 2017, 77, 67-73.	0.5	2
26	i /> Bulk Defect Chemistry of PCFC Cathode Materials: Discussion of Defect Interactions. <i>ECS Transactions</i> , 2017, 77, 133-138.	0.5	15
27	Mixed conductivity of polythiophene-based ionic polymers under controlled conditions. <i>Polymer</i> , 2017, 132, 216-226.	3.8	21
28	Proton uptake into the protonic cathode material BaCo _{0.4} Fe _{0.4} Zr _{0.2} O _{3-δ} and comparison to protonic electrolyte materials. <i>Solid State Ionics</i> , 2017, 299, 64-69.	2.7	82
29	Ab initio modelling of oxygen vacancies and protonic defects in La _x Sr _x FeO _{3-δ} perovskite solid solutions. <i>Journal of Materials Chemistry A</i> , 2016, 4, 13093-13104.	10.3	33
30	(Invited) Oxygen Reduction Reaction at Cathodes on Proton Conducting Oxide Electrolytes: Contribution from Three Phase Boundary Compared to Bulk Path. <i>ECS Transactions</i> , 2015, 66, 95-102.	0.5	14
31	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
32	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
33	Proton uptake in the H ⁺ -SOFC cathode material Ba _{0.5} Sr _{0.5} Fe _{0.8} Zn _{0.2} O _{3-δ} : transition from hydration to hydrogenation with increasing oxygen partial pressure. <i>Faraday Discussions</i> , 2015, 182, 129-143.	3.2	76
34	Proton conductivity in mixed-conducting BSFZ perovskite from thermogravimetric relaxation. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 16446.	2.8	89
35	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
36	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

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37	Formation and migration of oxygen vacancies in $\text{La}_{1-x}\text{Sr}_x\text{Co}_{1-y}\text{Fe}_y\text{O}_{3-\delta}$ perovskites: insight from ab initio calculations and comparison with $\text{Ba}_{1-x}\text{Sr}_x\text{Co}_{1-y}\text{Fe}_y\text{O}_{3-\delta}$. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 911-919.	2.8	111
38	Oxygen exchange kinetics on solid oxide fuel cell cathode materials—general trends and their mechanistic interpretation. <i>Journal of Materials Research</i> , 2012, 27, 2000-2008.	2.6	85
39	Nonlinear electrical grain boundary properties in proton conducting $\text{Y}\delta\text{-BaZrO}_3$ supporting the space charge depletion model. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 730-740.	2.8	90
40	Dopant Segregation and Space Charge Effects in Proton-Conducting BaZrO_3 Perovskites. <i>Journal of Physical Chemistry C</i> , 2012, 116, 2453-2461.	3.1	106
41	Long-Range and Short-Range Structure of Proton-Conducting Y:BaZrO_3 . <i>Chemistry of Materials</i> , 2011, 23, 2994-3002.	6.7	93
42	First Principles Calculations of Oxygen Vacancy Formation and Migration in $\text{Ba}_{1-x}\text{Sr}_x\text{Co}_{1-y}\text{Fe}_y\text{O}_{3-\delta}$ Perovskites. <i>Journal of the Electrochemical Society</i> , 2011, 159, B219-B226.	2.9	84
43	First principles calculations of oxygen vacancy formation and migration in mixed conducting $\text{Ba}_{0.5}\text{Sr}_{0.5}\text{Co}_{1-y}\text{Fe}_y\text{O}_{3-\delta}$ perovskites. <i>Solid State Ionics</i> , 2011, 188, 1-5.	2.7	98
44	Pathways for Oxygen Incorporation in Mixed Conducting Perovskites: A DFT-Based Mechanistic Analysis for $(\text{La}, \text{Sr})\text{MnO}_{3-\delta}$. <i>Journal of Physical Chemistry C</i> , 2010, 114, 3017-3027.	3.1	160
45	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
46	PLD-deposited $(\text{Ba}_x\text{Sr}_{1-x})(\text{Co}_y\text{Fe}_{1-y})\text{O}_{3-\delta}$ Thin-Film Microelectrodes: Structure Aspects and Oxygen Incorporation Kinetics. <i>ECS Transactions</i> , 2008, 13, 85-95.	0.5	14
47	The $p(\text{O}_2)$ dependence of oxygen surface coverage and exchange current density of mixed conducting oxide electrodes: model considerations. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 2713.	2.8	66
48	Jahn-Teller distortion around Fe^{4+} in $\text{Ba}_{1-x}\text{Sr}_x\text{Co}_{1-y}\text{Fe}_y\text{O}_{3-\delta}$ perovskites. <i>Physical Chemistry Chemical Physics</i> , 2007, 9, 2713.		