Karl T Mueller

List of Publications by Year
in descending order

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86 papers	5,874 citations	147801 31 h-index	74163 75 g-index
89 all docs	89 docs citations	89 times ranked	7073 citing authors

#	Article	IF	Citations
1	Solvation Structure and Dynamics of Mg(TFSI)₂ Aqueous Electrolyte. Energy and Environmental Materials, 2022, 5, 295-304.	12.8	19
2	Concentration-dependent ion correlations impact the electrochemical behavior of calcium battery electrolytes. Physical Chemistry Chemical Physics, 2022, 24, 674-686.	2.8	13
3	An automated framework for high-throughput predictions of NMR chemical shifts within liquid solutions. Nature Computational Science, 2022, 2, 112-122.	8.0	4
4	Understanding the Solvation-Dependent Properties of Cyclic Ether Multivalent Electrolytes Using High-Field NMR and Quantum Chemistry. Jacs Au, 2022, 2, 917-932.	7.9	5
5	A sobering examination of the feasibility of aqueous aluminum batteries. Energy and Environmental Science, 2022, 15, 2460-2469.	30.8	27
6	Factors Influencing Preferential Anion Interactions during Solvation of Multivalent Cations in Ethereal Solvents. Journal of Physical Chemistry C, 2021, 125, 6005-6012.	3.1	17
7	Quantifying Species Populations in Multivalent Borohydride Electrolytes. Journal of Physical Chemistry B, 2021, 125, 3644-3652.	2.6	17
8	Advancing Electrolyte Solution Chemistry and Interfacial Electrochemistry of Divalent Metal Batteries. ChemElectroChem, 2021, 8, 3013-3029.	3.4	13
9	Insights into Spontaneous Solid Electrolyte Interphase Formation at Magnesium Metal Anode Surface from Ab Initio Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2021, 13, 38816-38825.	8.0	20
10	Role of Polysulfide Anions in Solid-Electrolyte Interphase Formation at the Lithium Metal Surface in Liâ€“S Batteries. Journal of Physical Chemistry Letters, 2021, 12, 9360-9367.	4.6	13
11	Role of a Multivalent Ionâ€“Solvent Interaction on Restricted Mg²⁺ Diffusion in Dimethoxyethane Electrolytes. Journal of Physical Chemistry B, 2021, 125, 12574-12583.	2.6	7
12	Pulsed Field Gradient Nuclear Magnetic Resonance and Diffusion Analysis in Battery Research. Chemistry of Materials, 2021, 33, 8562-8590.	6.7	20
13	Reversible Electrochemical Interface of Mg Metal and Conventional Electrolyte Enabled by Intermediate Adsorption. ACS Energy Letters, 2020, 5, 200-206.	17.4	44
14	Mg²⁺ Diffusion-Induced Structural and Property Evolution in Epitaxial Fe₃O₄ Thin Films. ACS Nano, 2020, 14, 14887-14894.	14.6	6
15	Role of Solvent Rearrangement on Mg²⁺ Solvation Structures in Dimethoxyethane Solutions using Multimodal NMR Analysis. Journal of Physical Chemistry Letters, 2020, 11, 6443-6449.	4.6	27
16	Origin of Unusual Acidity and Li⁺ Diffusivity in a Series of Water-in-Salt Electrolytes. Journal of Physical Chemistry B, 2020, 124, 5284-5291.	2.6	26
17	Defect-induced anisotropic surface reactivity and ion transfer processes of anatase nanoparticles. Materials Today Chemistry, 2020, 17, 100290.	3.5	0
18	Energy storage emerging: A perspective from the Joint Center for Energy Storage Research. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 12550-12557.	7.1	218

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19	A lithium-sulfur battery with a solution-mediated pathway operating under lean electrolyte conditions. Nano Energy, 2020, 76, 105041.	16.0	25
20	Probing Conformational Evolution and Associated Dynamics of Mg(N(SO₂CF₃)₂)₂Â·Dimethoxyethane Adduct Using Solid-State ¹⁹F and ¹H NMR. Journal of Physical Chemistry C, 2020, 124, 4999-5008.	3.1	13
21	Variable Temperature and Pressure Operando MAS NMR for Catalysis Science and Related Materials. Accounts of Chemical Research, 2020, 53, 611-619.	15.6	48
22	Evolution of Ionâ€“Ion Interactions and Structures in Smectic Ionic Liquid Crystals. Journal of Physical Chemistry C, 2019, 123, 20547-20557.	3.1	8
23	Role of Inorganic Surface Layer on Solid Electrolyte Interphase Evolution at Li-Metal Anodes. ACS Applied Materials & Interfaces, 2019, 11, 31467-31476.	8.0	75
24	Mechanism by which Tungsten Oxide Promotes the Activity of Supported V₂O₅/TiO₂ Catalysts for NO_X Abatement: Structural Effects Revealed by ⁵¹V MAS NMR Spectroscopy. Angewandte Chemie - International Edition, 2019, 58, 12609-12616.	13.8	96
25	Mechanism by which Tungsten Oxide Promotes the Activity of Supported V₂O₅/TiO₂ Catalysts for NO_X Abatement: Structural Effects Revealed by ⁵¹V MAS NMR Spectroscopy. Angewandte Chemie, 2019, 131, 12739-12746.	2.0	45
26	Adsorption and Thermal Decomposition of Electrolytes on Nanometer Magnesium Oxide: An in Situ 13C MAS NMR Study. ACS Applied Materials & Interfaces, 2019, 11, 38689-38696.	8.0	19
27	The formation of Gluconacetobacter xylinum cellulose under the influence of the dye brilliant yellow. Cellulose, 2019, 26, 9373-9386.	4.9	2
28	A multi-functional interface derived from thiol-modified mesoporous carbon in lithiumâ€“sulfur batteries. Journal of Materials Chemistry A, 2019, 7, 13372-13381.	10.3	17
29	Monitoring solvent dynamics and ion associations in the formation of cubic octamer polyanion in tetramethylammonium silicate solutions. Physical Chemistry Chemical Physics, 2019, 21, 4717-4720.	2.8	9
30	Structure and Dynamics of Polysulfide Clusters in a Nonaqueous Solvent Mixture of 1,3-Dioxolane and 1,2-Dimethoxyethane. Chemistry of Materials, 2019, 31, 2308-2319.	6.7	54
31	Addressing Passivation in Lithiumâ€“Sulfur Battery Under Lean Electrolyte Condition. Advanced Functional Materials, 2018, 28, 1707234.	14.9	143
32	In situ and ex situ NMR for battery research. Journal of Physics Condensed Matter, 2018, 30, 463001.	1.8	35
33	Lean Electrolyte Batteries: Addressing Passivation in Lithiumâ€“Sulfur Battery Under Lean Electrolyte Condition (Adv. Funct. Mater. 38/2018). Advanced Functional Materials, 2018, 28, 1870275.	14.9	5
34	Calculations of solidâ€state ⁴³Ca NMR parameters: A comparison of periodic and cluster approaches and an evaluation of DFT functionals. Journal of Computational Chemistry, 2017, 38, 949-956.	3.3	19
35	Surface Interactions and Confinement of Methane: A High Pressure Magic Angle Spinning NMR and Computational Chemistry Study. Langmuir, 2017, 33, 1359-1367.	3.5	22
36	Semi-empirical refinements of crystal structures using 17O quadrupolar-coupling tensors. Journal of Chemical Physics, 2017, 146, 064201.	3.0	26

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37	In Situ Chemical Imaging of Solid-Electrolyte Interphase Layer Evolution in Liâ€“S Batteries. Chemistry of Materials, 2017, 29, 4728-4737.	6.7	147
38	Improving Lithiumâ€“Sulfur Battery Performance under Lean Electrolyte through Nanoscale Confinement in Soft Swellable Gels. Nano Letters, 2017, 17, 3061-3067.	9.1	122
39	Toward high-resolution NMR spectroscopy of microscopic liquid samples. Physical Chemistry Chemical Physics, 2017, 19, 14256-14261.	2.8	6
40	Multinuclear NMR Study of the Solid Electrolyte Interface Formed in Lithium Metal Batteries. ACS Applied Materials & Interfaces, 2017, 9, 14741-14748.	8.0	47
41	Elucidating the Solvation Structure and Dynamics of Lithium Polysulfides Resulting from Competitive Salt and Solvent Interactions. Chemistry of Materials, 2017, 29, 3375-3379.	6.7	117
42	Ammonium Additives to Dissolve Lithium Sulfide through Hydrogen Binding for High-Energy Lithiumâ€“Sulfur Batteries. ACS Applied Materials & Interfaces, 2017, 9, 4290-4295.	8.0	74
43	Imaging Electrochemical Processes in Li Batteries by Operando STEM. Microscopy and Microanalysis, 2017, 23, 1970-1971.	0.4	1
44	Fabrication of phosphonic acid films on nitinol nanoparticles by dynamic covalent assembly. Thin Solid Films, 2017, 642, 195-206.	1.8	12
45	Controlling Solidâ€“Liquid Conversion Reactions for a Highly Reversible Aqueous Zincâ€“Iodine Battery. ACS Energy Letters, 2017, 2, 2674-2680.	17.4	207
46	High-resolution microstrip NMR detectors for subnanoliter samples. Physical Chemistry Chemical Physics, 2017, 19, 28163-28174.	2.8	12
47	Non-encapsulation approach for high-performance Liâ€“S batteries through controlled nucleation and growth. Nature Energy, 2017, 2, 813-820.	39.5	326
48	Effects of Anion Mobility on Electrochemical Behaviors of Lithiumâ€“Sulfur Batteries. Chemistry of Materials, 2017, 29, 9023-9029.	6.7	35
49	Uranium Release from Acidic Weathered Hanford Sediments: Single-Pass Flow-Through and Column Experiments. Environmental Science & Technology, 2017, 51, 11011-11019.	10.0	15
50	Study of Perfluorophosphonic Acid Surface Modifications on Zinc Oxide Nanoparticles. Materials, 2017, 10, 1363.	2.9	27
51	Molecular Storage of Mg Ions with Vanadium Oxide Nanoclusters. Advanced Functional Materials, 2016, 26, 3446-3453.	14.9	65
52	Restricting the Solubility of Polysulfides in Liâ€S Batteries Via Electrolyte Salt Selection. Advanced Energy Materials, 2016, 6, 1600160.	19.5	66
53	Analysis of the bondâ€valence method for calculating 29 Si and 31 P magnetic shielding in covalent network solids. Journal of Computational Chemistry, 2016, 37, 1704-1710.	3.3	14
54	Effect of the Anion Activity on the Stability of Li Metal Anodes in Lithiumâ€Sulfur Batteries. Advanced Functional Materials, 2016, 26, 3059-3066.	14.9	117

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55	Diffusive Flux as a New Metric for Ion-Conducting Soft Materials. ACS Energy Letters, 2016, 1, 1179-1183.	17.4	15
56	The diffusion and conduction of lithium in poly(ethylene oxide)-based sulfonate ionomers. Journal of Chemical Physics, 2016, 145, 114903.	3.0	17
57	Facilitated Ion Transport in Smectic Ordered Ionic Liquid Crystals. Advanced Materials, 2016, 28, 9301-9307.	21.0	36
58	Reversible aqueous zinc/manganese oxide energy storage from conversion reactions. Nature Energy, 2016, 1, .	39.5	2,186
59	Preferential Solvation of an Asymmetric Redox Molecule. Journal of Physical Chemistry C, 2016, 120, 27834-27839.	3.1	18
60	Liquid Crystals: Facilitated Ion Transport in Smectic Ordered Ionic Liquid Crystals (Adv. Mater.) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 542	21.0	1
61	The Impact of Li Grain Size on Coulombic Efficiency in Li Batteries. Scientific Reports, 2016, 6, 34267.	3.3	67
62	Understanding the Effect of Additives in Li-ion and Li-Sulfur Batteries by Operando ec- (S)TEM. Microscopy and Microanalysis, 2016, 22, 22-23.	0.4	5
63	Nuclear magnetic resonance studies of the solvation structures of a high-performance nonaqueous redox flow electrolyte. Journal of Power Sources, 2016, 308, 172-179.	7.8	15
64	Sustainable development of a surface-functionalized mesoporous aluminosilicate with ultra-high ion exchange efficiency. Inorganic Chemistry Frontiers, 2016, 3, 502-513.	6.0	23
65	Monitoring the refinement of crystal structures with 15N solid-state NMR shift tensor data. Journal of Chemical Physics, 2015, 143, 194702.	3.0	31
66	Nanocomposite polymer electrolyte for rechargeable magnesium batteries. Nano Energy, 2015, 12, 750-759.	16.0	121
67	Critical Analysis of Cluster Models and Exchange-Correlation Functionals for Calculating Magnetic Shielding in Molecular Solids. Journal of Chemical Theory and Computation, 2015, 11, 5229-5241.	5.3	60
68	Solvation structure and transport properties of alkali cations in dimethyl sulfoxide under exogenous static electric fields. Journal of Chemical Physics, 2015, 142, 224502.	3.0	12
69	Experiences with a researcher-centric ELN. Chemical Science, 2015, 6, 1614-1629.	7.4	24
70	Density functional investigation of intermolecular effects on 13C NMR chemical-shielding tensors modeled with molecular clusters. Journal of Chemical Physics, 2014, 141, 164121.	3.0	53
71	Diffusional motion of redox centers in carbonate electrolytes. Journal of Chemical Physics, 2014, 141, 104509.	3.0	24
72	Solid state nuclear magnetic resonance investigation of polymer backbone dynamics in poly(ethylene) Tj ETQq0 0 0 rgBT /Overlock 10 T 2013, 138, 194907.	3.0	9

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73	Nuclear magnetic resonance investigation of dynamics in poly(ethylene oxide)-based lithium polyether-ester-sulfonate ionomers. Journal of Chemical Physics, 2012, 136, 014510.	3.0	25
74	Effect of SiO2 on Densification and Microstructure Development in Nd:YAG Transparent Ceramics. Journal of the American Ceramic Society, 2011, 94, 1380-1387.	3.8	130
75	Cesium and strontium incorporation into zeolite-type phases during homogeneous nucleation from caustic solutions. American Mineralogist, 2011, 96, 1809-1820.	1.9	11
76	Description of Mg²⁺ Release from Forsterite Using Ab Initio Methods. Journal of Physical Chemistry C, 2010, 114, 5417-5428.	3.1	20
77	Characterization of cation environments in polycrystalline forsterite by 25Mg MAS, MQMAS, and QCPMG NMR. American Mineralogist, 2010, 95, 1601-1607.	1.9	10
78	Intermolecular shielding contributions studied by modeling the C13 chemical-shift tensors of organic single crystals with plane waves. Journal of Chemical Physics, 2009, 131, 144503.	3.0	75
79	Silicon control of strontium and cesium partitioning in hydroxide-weathered sediments. Geochimica Et Cosmochimica Acta, 2008, 72, 2024-2047.	3.9	54
80	Investigation of Lead Borosilicate Glass Structure With 207Pb and 11B Solid-State NMR. Materials Research Society Symposia Proceedings, 2000, 658, 3221.	0.1	0
81	Determination of internuclear distances from solid-state nuclear magnetic resonance: Dipolar transforms and regularization methods. Molecular Physics, 1998, 95, 907-919.	1.7	22
82	Determination of internuclear distances from solid-state nuclear magnetic resonance: dipolar transforms and regularization methods. Molecular Physics, 1998, 95, 907-919.	1.7	3
83	Synthesis of Porous Transition Metal Oxides by the Salt-Gel Method. Materials Research Society Symposia Proceedings, 1994, 371, 69.	0.1	6
84	High-resolution oxygen-17 NMR of solid silicates. Journal of the American Chemical Society, 1991, 113, 32-38.	13.7	120
85	Dynamic-angle spinning of quadrupolar nuclei. Journal of Magnetic Resonance, 1990, 86, 470-487.	0.5	106
86	Modelling complex molecular interactions in catalytic materials for energy storage and conversion in nuclear magnetic resonance. Frontiers in Catalysis, 0, 2, .	3.9	1