Karl T Mueller

List of Publications by Citations

85 papers	3,982 citations	28 h-index	62 g-index
89 ext. papers	4,872 ext. citations	9.9 avg, IF	5.29 L-index

#	Paper	IF	Citations
85	Reversible aqueous zinc/manganese oxide energy storage from conversion reactions. *Nature Energy*, **2016**, 1,	62.3	1461
84	Non-encapsulation approach for high-performance Li–S batteries through controlled nucleation and growth. *Nature Energy*, **2017**, 2, 813-820	62.3	256
83	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	113
82	Addressing Passivation in Lithium–Sulfur Battery Under Lean Electrolyte Condition. *Advanced Functional Materials*, **2018**, 28, 1707234	15.6	111
81	High-resolution oxygen-17 NMR of solid silicates. *Journal of the American Chemical Society*, **1991**, 113, 32-38	16.4	104
80	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	11.5	103
79	Improving Lithium-Sulfur Battery Performance under Lean Electrolyte through Nanoscale Confinement in Soft Swellable Gels. *Nano Letters*, **2017**, 17, 3061-3067	11.5	99
78	In Situ Chemical Imaging of Solid-Electrolyte Interphase Layer Evolution in Li–S Batteries. *Chemistry of Materials*, **2017**, 29, 4728-4737	9.6	98
77	Controlling Solid–Liquid Conversion Reactions for a Highly Reversible Aqueous Zinc–Iodine Battery. *ACS Energy Letters*, **2017**, 2, 2674-2680	20.1	96
76	Effect of the Anion Activity on the Stability of Li Metal Anodes in Lithium-Sulfur Batteries. *Advanced Functional Materials*, **2016**, 26, 3059-3066	15.6	89
75	Nanocomposite polymer electrolyte for rechargeable magnesium batteries. *Nano Energy*, **2015**, 12, 750-759	17.1	86
74	Elucidating the Solvation Structure and Dynamics of Lithium Polysulfides Resulting from Competitive Salt and Solvent Interactions. *Chemistry of Materials*, **2017**, 29, 3375-3379	9.6	78
73	Intermolecular shielding contributions studied by modeling the (13)C chemical-shift tensors of organic single crystals with plane waves. *Journal of Chemical Physics*, **2009**, 131, 144503	3.9	71
72	Dynamic-angle spinning of quadrupolar nuclei. *Journal of Magnetic Resonance*, **1990**, 86, 470-487		58
71	Restricting the Solubility of Polysulfides in Li-S Batteries Via Electrolyte Salt Selection. *Advanced Energy Materials*, **2016**, 6, 1600160	21.8	57
70	The Impact of Li Grain Size on Coulombic Efficiency in Li Batteries. *Scientific Reports*, **2016**, 6, 34267	4.9	53
69	Ammonium Additives to Dissolve Lithium Sulfide through Hydrogen Binding for High-Energy Lithium-Sulfur Batteries. *ACS Applied Materials & Interfaces*, **2017**, 9, 4290-4295	9.5	51

68	Molecular Storage of Mg Ions with Vanadium Oxide Nanoclusters. *Advanced Functional Materials*, **2016**, 26, 3446-3453	15.6	50
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, 5229-41	6.4	49
66	Mechanism by which Tungsten Oxide Promotes the Activity of Supported V O /TiO Catalysts for NO Abatement: Structural Effects Revealed by V MAS NMR Spectroscopy. *Angewandte Chemie - International Edition*, **2019**, 58, 12609-12616	16.4	48
65	Silicon control of strontium and cesium partitioning in hydroxide-weathered sediments. *Geochimica Et Cosmochimica Acta*, **2008**, 72, 2024-2047	5.5	48
64	Role of Inorganic Surface Layer on Solid Electrolyte Interphase Evolution at Li-Metal Anodes. *ACS Applied Materials & Interfaces*, **2019**, 11, 31467-31476	9.5	47
63	Density functional investigation of intermolecular effects on 13C NMR chemical-shielding tensors modeled with molecular clusters. *Journal of Chemical Physics*, **2014**, 141, 164121	3.9	47
62	Multinuclear NMR Study of the Solid Electrolyte Interface Formed in Lithium Metal Batteries. *ACS Applied Materials & Interfaces*, **2017**, 9, 14741-14748	9.5	36
61	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	9.6	36
60	Variable Temperature and Pressure Operando MAS NMR for Catalysis Science and Related Materials. *Accounts of Chemical Research*, **2020**, 53, 611-619	24.3	30
59	Mechanism by which Tungsten Oxide Promotes the Activity of Supported V2O5/TiO2 Catalysts for NOX Abatement: Structural Effects Revealed by 51V MAS NMR Spectroscopy. *Angewandte Chemie*, **2019**, 131, 12739-12746	3.6	30
58	Facilitated Ion Transport in Smectic Ordered Ionic Liquid Crystals. *Advanced Materials*, **2016**, 28, 9301-9307	24	29
57	Effects of Anion Mobility on Electrochemical Behaviors of Lithium-Sulfur Batteries. *Chemistry of Materials*, **2017**, 29, 9023-9029	9.6	28
56	Monitoring the refinement of crystal structures with (15)N solid-state NMR shift tensor data. *Journal of Chemical Physics*, **2015**, 143, 194702	3.9	26
55	In situ and ex situ NMR for battery research. *Journal of Physics Condensed Matter*, **2018**, 30, 463001	1.8	22
54	Diffusional motion of redox centers in carbonate electrolytes. *Journal of Chemical Physics*, **2014**, 141, 104509	3.9	21
53	Nuclear magnetic resonance investigation of dynamics in poly(ethylene oxide)-based lithium polyether-ester-sulfonate ionomers. *Journal of Chemical Physics*, **2012**, 136, 014510	3.9	20
52	Determination of internuclear distances from solid-state nuclear magnetic resonance: Dipolar transforms and regularization methods. *Molecular Physics*, **1998**, 95, 907-919	1.7	20
51	Calculations of solid-state Ca NMR parameters: A comparison of periodic and cluster approaches and an evaluation of DFT functionals. *Journal of Computational Chemistry*, **2017**, 38, 949-956	3.5	18

50	Semi-empirical refinements of crystal structures using O quadrupolar-coupling tensors. *Journal of Chemical Physics*, **2017**, 146, 064201	3.9	18
49	Experiences with a researcher-centric ELN. *Chemical Science*, **2015**, 6, 1614-1629	9.4	18
48	Sustainable development of a surface-functionalized mesoporous aluminosilicate with ultra-high ion exchange efficiency. *Inorganic Chemistry Frontiers*, **2016**, 3, 502-513	6.8	17
47	Study of Perfluorophosphonic Acid Surface Modifications on Zinc Oxide Nanoparticles. *Materials*, **2017**, 10,	3.5	17
46	Reversible Electrochemical Interface of Mg Metal and Conventional Electrolyte Enabled by Intermediate Adsorption. *ACS Energy Letters*, **2020**, 5, 200-206	20.1	17
45	Surface Interactions and Confinement of Methane: A High Pressure Magic Angle Spinning NMR and Computational Chemistry Study. *Langmuir*, **2017**, 33, 1359-1367	4	16
44	Nuclear magnetic resonance studies of the solvation structures of a high-performance nonaqueous redox flow electrolyte. *Journal of Power Sources*, **2016**, 308, 172-179	8.9	15
43	Description of Mg2+ Release from Forsterite Using Ab Initio Methods *Journal of Physical Chemistry C*, **2010**, 114, 5417-5428	3.8	15
42	Origin of Unusual Acidity and Li Diffusivity in a Series of Water-in-Salt Electrolytes. *Journal of Physical Chemistry B*, **2020**, 124, 5284-5291	3.4	14
41	A lithium-sulfur battery with a solution-mediated pathway operating under lean electrolyte conditions. *Nano Energy*, **2020**, 76, 105041	17.1	14
40	Analysis of the bond-valence method for calculating (29) Si and (31) P magnetic shielding in covalent network solids. *Journal of Computational Chemistry*, **2016**, 37, 1704-10	3.5	13
39	Adsorption and Thermal Decomposition of Electrolytes on Nanometer Magnesium Oxide: An in Situ C MAS NMR Study. *ACS Applied Materials & Interfaces*, **2019**, 11, 38689-38696	9.5	12
38	Preferential Solvation of an Asymmetric Redox Molecule. *Journal of Physical Chemistry C*, **2016**, 120, 27834-27839	3.8	12
37	Role of Solvent Rearrangement on Mg Solvation Structures in Dimethoxyethane Solutions using Multimodal NMR Analysis. *Journal of Physical Chemistry Letters*, **2020**, 11, 6443-6449	6.4	12
36	The diffusion and conduction of lithium in poly(ethylene oxide)-based sulfonate ionomers. *Journal of Chemical Physics*, **2016**, 145, 114903	3.9	12
35	A multi-functional interface derived from thiol-modified mesoporous carbon in lithium–sulfur batteries. *Journal of Materials Chemistry A*, **2019**, 7, 13372-13381	13	11
34	Uranium Release from Acidic Weathered Hanford Sediments: Single-Pass Flow-Through and Column Experiments. *Environmental Science & Technology*, **2017**, 51, 11011-11019	10.3	11
33	Diffusive Flux as a New Metric for Ion-Conducting Soft Materials. *ACS Energy Letters*, **2016**, 1, 1179-1183	20.1	11

32	Characterization of cation environments in polycrystalline forsterite by 25Mg MAS, MQMAS, and QCPMG NMR. *American Mineralogist*, **2010**, 95, 1601-1607	2.9	10
31	Fabrication of phosphonic acid films on nitinol nanoparticles by dynamic covalent assembly. *Thin Solid Films*, **2017**, 642, 195-206	2.2	8
30	High-resolution microstrip NMR detectors for subnanoliter samples. *Physical Chemistry Chemical Physics*, **2017**, 19, 28163-28174	3.6	8
29	Solvation structure and transport properties of alkali cations in dimethyl sulfoxide under exogenous static electric fields. *Journal of Chemical Physics*, **2015**, 142, 224502	3.9	8
28	Solid state nuclear magnetic resonance investigation of polymer backbone dynamics in poly(ethylene oxide) based lithium and sodium polyether-ester-sulfonate ionomers. *Journal of Chemical Physics*, **2013**, 138, 194907	3.9	8
27	Cesium and strontium incorporation into zeolite-type phases during homogeneous nucleation from caustic solutions. *American Mineralogist*, **2011**, 96, 1809-1820	2.9	8
26	Factors Influencing Preferential Anion Interactions during Solvation of Multivalent Cations in Ethereal Solvents. *Journal of Physical Chemistry C*, **2021**, 125, 6005-6012	3.8	8
25	Quantifying Species Populations in Multivalent Borohydride Electrolytes. *Journal of Physical Chemistry B*, **2021**, 125, 3644-3652	3.4	7
24	Probing Conformational Evolution and Associated Dynamics of Mg(N(SO2CF3)2)2□Dimethoxyethane Adduct Using Solid-State 19F and 1H NMR. *Journal of Physical Chemistry C*, **2020**, 124, 4999-5008	3.8	6
23	Evolution of Ion□bn Interactions and Structures in Smectic Ionic Liquid Crystals. *Journal of Physical Chemistry C*, **2019**, 123, 20547-20557	3.8	6
22	Solvation Structure and Dynamics of Mg(TFSI)2 Aqueous Electrolyte. *Energy and Environmental Materials*,	13	6
21	Understanding the Effect of Additives in Li-ion and Li-Sulfur Batteries by Operando ec- (S)TEM. *Microscopy and Microanalysis*, **2016**, 22, 22-23	0.5	5
20	Synthesis of Porous Transition Metal Oxides by the Salt-Gel Method. *Materials Research Society Symposia Proceedings*, **1994**, 371, 69		5
19	Lean Electrolyte Batteries: Addressing Passivation in Lithium□Sulfur Battery Under Lean Electrolyte Condition (Adv. Funct. Mater. 38/2018). *Advanced Functional Materials*, **2018**, 28, 1870275	15.6	5
18	Toward high-resolution NMR spectroscopy of microscopic liquid samples. *Physical Chemistry Chemical Physics*, **2017**, 19, 14256-14261	3.6	4
17	Role of a Multivalent Ion-Solvent Interaction on Restricted Mg Diffusion in Dimethoxyethane Electrolytes. *Journal of Physical Chemistry B*, **2021**, 125, 12574-12583	3.4	4
16	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	3.6	4
15	Concentration-dependent ion correlations impact the electrochemical behavior of calcium battery electrolytes.. *Physical Chemistry Chemical Physics*, **2021**,	3.6	3

14	Pulsed Field Gradient Nuclear Magnetic Resonance and Diffusion Analysis in Battery Research. *Chemistry of Materials*, **2021**, 33, 8562-8590	9.6	3
13	Determination of internuclear distances from solid-state nuclear magnetic resonance: Dipolar transforms and regularization methods		3
12	Mg Diffusion-Induced Structural and Property Evolution in Epitaxial FeO Thin Films. *ACS Nano*, **2020**, 14, 14887-14894	16.7	3
11	Insights into Spontaneous Solid Electrolyte Interphase Formation at Magnesium Metal Anode Surface from Molecular Dynamics Simulations. *ACS Applied Materials & Interfaces*, **2021**, 13, 38816-38825	9.5	3
10	Computational Spectroscopy in Environmental Chemistry **2010**, 323-351		2
9	Advancing Electrolyte Solution Chemistry and Interfacial Electrochemistry of Divalent Metal Batteries. *ChemElectroChem*, **2021**, 8, 3013-3029	4.3	2
8	Imaging Electrochemical Processes in Li Batteries by Operando STEM. *Microscopy and Microanalysis*, **2017**, 23, 1970-1971	0.5	1
7	The formation of Gluconacetobacter xylinum cellulose under the influence of the dye brilliant yellow. *Cellulose*, **2019**, 26, 9373-9386	5.5	1
6	Liquid Crystals: Facilitated Ion Transport in Smectic Ordered Ionic Liquid Crystals (Adv. Mater. 42/2016). *Advanced Materials*, **2016**, 28, 9439-9439	24	1
5	Role of Polysulfide Anions in Solid-Electrolyte Interphase Formation at the Lithium Metal Surface in Li-S Batteries. *Journal of Physical Chemistry Letters*, **2021**, 12, 9360-9367	6.4	1
4	Understanding the Solvation-Dependent Properties of Cyclic Ether Multivalent Electrolytes Using High-Field NMR and Quantum Chemistry.. *Jacs Au*, **2022**, 2, 917-932		1
3	An automated framework for high-throughput predictions of NMR chemical shifts within liquid solutions. *Nature Computational Science*, **2022**, 2, 112-122		0
2	Defect-induced anisotropic surface reactivity and ion transfer processes of anatase nanoparticles. *Materials Today Chemistry*, **2020**, 17, 100290	6.2	
1	Investigation of Lead Borosilicate Glass Structure With 207Pb and 11B Solid-State NMR. *Materials Research Society Symposia Proceedings*, **2000**, 658, 3221		