## Karl T Mueller

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Reversible aqueous zinc/manganese oxide energy storage from conversion reactions. Nature Energy, 2016, 1, .	39.5	2,186
2	Non-encapsulation approach for high-performance Li–S batteries through controlled nucleation and growth. Nature Energy, 2017, 2, 813-820.	39.5	326
3	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
4	Controlling Solid–Liquid Conversion Reactions for a Highly Reversible Aqueous Zinc–lodine Battery. ACS Energy Letters, 2017, 2, 2674-2680.	17.4	207
5	In Situ Chemical Imaging of Solid-Electrolyte Interphase Layer Evolution in Li–S Batteries. Chemistry of Materials, 2017, 29, 4728-4737.	6.7	147
6	Addressing Passivation in Lithium–Sulfur Battery Under Lean Electrolyte Condition. Advanced Functional Materials, 2018, 28, 1707234.	14.9	143
7	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
8	Improving Lithium–Sulfur Battery Performance under Lean Electrolyte through Nanoscale Confinement in Soft Swellable Gels. Nano Letters, 2017, 17, 3061-3067.	9.1	122
9	Nanocomposite polymer electrolyte for rechargeable magnesium batteries. Nano Energy, 2015, 12, 750-759.	16.0	121
10	High-resolution oxygen-17 NMR of solid silicates. Journal of the American Chemical Society, 1991, 113, 32-38.	13.7	120
11	Effect of the Anion Activity on the Stability of Li Metal Anodes in Lithiumâ€6ulfur Batteries. Advanced Functional Materials, 2016, 26, 3059-3066.	14.9	117
12	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
13	Dynamic-angle spinning of quadrupolar nuclei. Journal of Magnetic Resonance, 1990, 86, 470-487.	O.5	106
14	Mechanism by which Tungsten Oxide Promotes the Activity of Supported V <sub>2</sub> O <sub>5</sub> /TiO <sub>2</sub> Catalysts for NO <sub><i>X</i></sub> Abatement: Structural Effects Revealed by <sup>51</sup> V MAS NMR Spectroscopy. Angewandte Chemie - International Edition, 2019, 58, 12609-12616.	13.8	96
15	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
16	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
17	Ammonium Additives to Dissolve Lithium Sulfide through Hydrogen Binding for High-Energy Lithium–Sulfur Batteries. ACS Applied Materials & Interfaces, 2017, 9, 4290-4295.	8.0	74
18	The Impact of Li Grain Size on Coulombic Efficiency in Li Batteries. Scientific Reports, 2016, 6, 34267.	3.3	67

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19	Restricting the Solubility of Polysulfides in Liâ€& Batteries Via Electrolyte Salt Selection. Advanced Energy Materials, 2016, 6, 1600160.	19.5	66
20	Molecular Storage of Mg Ions with Vanadium Oxide Nanoclusters. Advanced Functional Materials, 2016, 26, 3446-3453.	14.9	65
21	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
22	Silicon control of strontium and cesium partitioning in hydroxide-weathered sediments. Geochimica Et Cosmochimica Acta, 2008, 72, 2024-2047.	3.9	54
23	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
24	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
25	Variable Temperature and Pressure Operando MAS NMR for Catalysis Science and Related Materials. Accounts of Chemical Research, 2020, 53, 611-619.	15.6	48
26	Multinuclear NMR Study of the Solid Electrolyte Interface Formed in Lithium Metal Batteries. ACS Applied Materials & Interfaces, 2017, 9, 14741-14748.	8.0	47
27	Mechanism by which Tungsten Oxide Promotes the Activity of Supported V <sub>2</sub> O <sub>5</sub> /TiO <sub>2</sub> Catalysts for NO <sub><i>X</i></sub> Abatement: Structural Effects Revealed by <sup>51</sup> V MAS NMR Spectroscopy. Angewandte Chemie, 2019, 131, 12739-12746.	2.0	45
28	Reversible Electrochemical Interface of Mg Metal and Conventional Electrolyte Enabled by Intermediate Adsorption. ACS Energy Letters, 2020, 5, 200-206.	17.4	44
29	Facilitated Ion Transport in Smectic Ordered Ionic Liquid Crystals. Advanced Materials, 2016, 28, 9301-9307.	21.0	36
30	Effects of Anion Mobility on Electrochemical Behaviors of Lithium–Sulfur Batteries. Chemistry of Materials, 2017, 29, 9023-9029.	6.7	35
31	<i>In situ</i> and <i>ex situ</i> NMR for battery research. Journal of Physics Condensed Matter, 2018, 30, 463001.	1.8	35
32	Monitoring the refinement of crystal structures with 15N solid-state NMR shift tensor data. Journal of Chemical Physics, 2015, 143, 194702.	3.0	31
33	Study of Perfluorophosphonic Acid Surface Modifications on Zinc Oxide Nanoparticles. Materials, 2017, 10, 1363.	2.9	27
34	Role of Solvent Rearrangement on Mg <sup>2+</sup> Solvation Structures in Dimethoxyethane Solutions using Multimodal NMR Analysis. Journal of Physical Chemistry Letters, 2020, 11, 6443-6449.	4.6	27
35	A sobering examination of the feasibility of aqueous aluminum batteries. Energy and Environmental Science, 2022, 15, 2460-2469.	30.8	27
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	Origin of Unusual Acidity and Li <sup>+</sup> Diffusivity in a Series of Water-in-Salt Electrolytes. Journal of Physical Chemistry B, 2020, 124, 5284-5291.	2.6	26
38	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
39	A lithium-sulfur battery with a solution-mediated pathway operating under lean electrolyte conditions. Nano Energy, 2020, 76, 105041.	16.0	25
40	Diffusional motion of redox centers in carbonate electrolytes. Journal of Chemical Physics, 2014, 141, 104509.	3.0	24
41	Experiences with a researcher-centric ELN. Chemical Science, 2015, 6, 1614-1629.	7.4	24
42	Sustainable development of a surface-functionalized mesoporous aluminosilicate with ultra-high ion exchange efficiency. Inorganic Chemistry Frontiers, 2016, 3, 502-513.	6.0	23
43	Determination of internuclear distances from solid-state nuclear magnetic resonance: Dipolar transforms and regularization methods. Molecular Physics, 1998, 95, 907-919.	1.7	22
44	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
45	Description of Mg <sup>2+</sup> Release from Forsterite Using Ab Initio Methods. Journal of Physical Chemistry C, 2010, 114, 5417-5428.	3.1	20
46	Insights into Spontaneous Solid Electrolyte Interphase Formation at Magnesium Metal Anode Surface from <i>Ab Initio</i> Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2021, 13, 38816-38825.	8.0	20
47	Pulsed Field Gradient Nuclear Magnetic Resonance and Diffusion Analysis in Battery Research. Chemistry of Materials, 2021, 33, 8562-8590.	6.7	20
48	Calculations of solidâ€state <sup>43</sup> Ca NMR parameters: A comparison of periodic and cluster approaches and an evaluation of DFT functionals. Journal of Computational Chemistry, 2017, 38, 949-956.	3.3	19
49	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
50	Solvation Structure and Dynamics of Mg(TFSI) <sub>2</sub> Aqueous Electrolyte. Energy and Environmental Materials, 2022, 5, 295-304.	12.8	19
51	Preferential Solvation of an Asymmetric Redox Molecule. Journal of Physical Chemistry C, 2016, 120, 27834-27839.	3.1	18
52	The diffusion and conduction of lithium in poly(ethylene oxide)-based sulfonate ionomers. Journal of Chemical Physics, 2016, 145, 114903.	3.0	17
53	A multi-functional interface derived from thiol-modified mesoporous carbon in lithium–sulfur batteries. Journal of Materials Chemistry A, 2019, 7, 13372-13381.	10.3	17
54	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

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55	Quantifying Species Populations in Multivalent Borohydride Electrolytes. Journal of Physical Chemistry B, 2021, 125, 3644-3652.	2.6	17
56	Diffusive Flux as a New Metric for Ion-Conducting Soft Materials. ACS Energy Letters, 2016, 1, 1179-1183.	17.4	15
57	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
58	Uranium Release from Acidic Weathered Hanford Sediments: Single-Pass Flow-Through and Column Experiments. Environmental Science & Technology, 2017, 51, 11011-11019.	10.0	15
59	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
60	Probing Conformational Evolution and Associated Dynamics of Mg(N(SO <sub>2</sub> CF <sub>3</sub> ) <sub>2</sub> ) <sub>2</sub> ·Dimethoxyethane Adduct Using Solid-State <sup>19</sup> F and <sup>1</sup> H NMR. Journal of Physical Chemistry C, 2020, 124, 4999-5008.	3.1	13
61	Advancing Electrolyte Solution Chemistry and Interfacial Electrochemistry of Divalent Metal Batteries. ChemElectroChem, 2021, 8, 3013-3029.	3.4	13
62	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.	4.6	13
63	Concentration-dependent ion correlations impact the electrochemical behavior of calcium battery electrolytes. Physical Chemistry Chemical Physics, 2022, 24, 674-686.	2.8	13
64	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
65	Fabrication of phosphonic acid films on nitinol nanoparticles by dynamic covalent assembly. Thin Solid Films, 2017, 642, 195-206.	1.8	12
66	High-resolution microstrip NMR detectors for subnanoliter samples. Physical Chemistry Chemical Physics, 2017, 19, 28163-28174.	2.8	12
67	Cesium and strontium incorporation into zeolite-type phases during homogeneous nucleation from caustic solutions. American Mineralogist, 2011, 96, 1809-1820.	1.9	11
68	Characterization of cation environments in polycrystalline forsterite by 25Mg MAS, MQMAS, and QCPMG NMR. American Mineralogist, 2010, 95, 1601-1607.	1.9	10
69	Solid state nuclear magnetic resonance investigation of polymer backbone dynamics in poly(ethylene) Tj ETQq1 2013, 138, 194907.	1 0.78431 3.0	4 rgBT /Ove 9
70	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
71	Evolution of Ion–Ion Interactions and Structures in Smectic Ionic Liquid Crystals. Journal of Physical Chemistry C, 2019, 123, 20547-20557.	3.1	8
72	Role of a Multivalent Ion–Solvent Interaction on Restricted Mg <sup>2+</sup> Diffusion in Dimethoxyethane Electrolytes. Journal of Physical Chemistry B, 2021, 125, 12574-12583.	2.6	7

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73	Synthesis of Porous Transition Metal Oxides by the Salt-Gel Method. Materials Research Society Symposia Proceedings, 1994, 371, 69.	0.1	6
74	Toward high-resolution NMR spectroscopy of microscopic liquid samples. Physical Chemistry Chemical Physics, 2017, 19, 14256-14261.	2.8	6
75	Mg <sup>2+</sup> Diffusion-Induced Structural and Property Evolution in Epitaxial Fe <sub>3</sub> O <sub>4</sub> Thin Films. ACS Nano, 2020, 14, 14887-14894.	14.6	6
76	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
77	Lean Electrolyte Batteries: Addressing Passivation in Lithium–Sulfur Battery Under Lean Electrolyte Condition (Adv. Funct. Mater. 38/2018). Advanced Functional Materials, 2018, 28, 1870275.	14.9	5
78	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
79	An automated framework for high-throughput predictions of NMR chemical shifts within liquid solutions. Nature Computational Science, 2022, 2, 112-122.	8.0	4
80	Determination of internuclear distances from solid-state nuclear magnetic resonance: dipolar transforms and regularization methods. Molecular Physics, 1998, 95, 907-919.	1.7	3
81	The formation of Gluconacetobacter xylinum cellulose under the influence of the dye brilliant yellow. Cellulose, 2019, 26, 9373-9386.	4.9	2
82	Liquid Crystals: Facilitated Ion Transport in Smectic Ordered Ionic Liquid Crystals (Adv. Mater.) Tj ETQq0 0 0 rgBT	Overlock	10 Tf 50 382

83	Imaging Electrochemical Processes in Li Batteries by Operando STEM. Microscopy and Microanalysis, 2017, 23, 1970-1971.	0.4	1
84	Modelling complex molecular interactions in catalytic materials for energy storage and conversion in nuclear magnetic resonance. Frontiers in Catalysis, 0, 2, .	3.9	1
85	Investigation of Lead Borosilicate Glass Structure With 207Pb and 11B Solid-State NMR. Materials Research Society Symposia Proceedings, 2000, 658, 3221.	0.1	0
86	Defect-induced anisotropic surface reactivity and ion transfer processes of anatase nanoparticles.	3.5	0

<sup>86</sup> Materials Today Chemistry, 2020, 17, 100290.