

Karl T Mueller

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	An automated framework for high-throughput predictions of NMR chemical shifts within liquid solutions. <i>Nature Computational Science</i> , 2022 , 2, 112-122		0
84	Understanding the Solvation-Dependent Properties of Cyclic Ether Multivalent Electrolytes Using High-Field NMR and Quantum Chemistry.. <i>Jacs Au</i> , 2022 , 2, 917-932		1
83	Concentration-dependent ion correlations impact the electrochemical behavior of calcium battery electrolytes.. <i>Physical Chemistry Chemical Physics</i> , 2021 ,	3.6	3
82	Role of a Multivalent Ion-Solvent Interaction on Restricted Mg Diffusion in Dimethoxyethane Electrolytes. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 12574-12583	3.4	4
81	Pulsed Field Gradient Nuclear Magnetic Resonance and Diffusion Analysis in Battery Research. <i>Chemistry of Materials</i> , 2021 , 33, 8562-8590	9.6	3
80	Factors Influencing Preferential Anion Interactions during Solvation of Multivalent Cations in Ethereal Solvents. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 6005-6012	3.8	8
79	Quantifying Species Populations in Multivalent Borohydride Electrolytes. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 3644-3652	3.4	7
78	Advancing Electrolyte Solution Chemistry and Interfacial Electrochemistry of Divalent Metal Batteries. <i>ChemElectroChem</i> , 2021 , 8, 3013-3029	4.3	2
77	Insights into Spontaneous Solid Electrolyte Interphase Formation at Magnesium Metal Anode Surface from Molecular Dynamics Simulations. <i>ACS Applied Materials & Interfaces</i> , 2021 , 13, 38816-38825	9.5	3
76	Role of Polysulfide Anions in Solid-Electrolyte Interphase Formation at the Lithium Metal Surface in Li-S Batteries. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 9360-9367	6.4	1
75	Origin of Unusual Acidity and Li Diffusivity in a Series of Water-in-Salt Electrolytes. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 5284-5291	3.4	14
74	Defect-induced anisotropic surface reactivity and ion transfer processes of anatase nanoparticles. <i>Materials Today Chemistry</i> , 2020 , 17, 100290	6.2	
73	Energy storage emerging: A perspective from the Joint Center for Energy Storage Research. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020 , 117, 12550-12557	11.5	103
72	A lithium-sulfur battery with a solution-mediated pathway operating under lean electrolyte conditions. <i>Nano Energy</i> , 2020 , 76, 105041	17.1	14
71	Probing Conformational Evolution and Associated Dynamics of Mg(N(SO ₂ CF ₃) ₂) ₂ Dimethoxyethane Adduct Using Solid-State ¹⁹ F and ¹ H NMR. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 4999-5008	3.8	6
70	Variable Temperature and Pressure Operando MAS NMR for Catalysis Science and Related Materials. <i>Accounts of Chemical Research</i> , 2020 , 53, 611-619	24.3	30
69	Reversible Electrochemical Interface of Mg Metal and Conventional Electrolyte Enabled by Intermediate Adsorption. <i>ACS Energy Letters</i> , 2020 , 5, 200-206	20.1	17

68	Mg Diffusion-Induced Structural and Property Evolution in Epitaxial FeO Thin Films. <i>ACS Nano</i> , 2020 , 14, 14887-14894	16.7	3
67	Role of Solvent Rearrangement on Mg Solvation Structures in Dimethoxyethane Solutions using Multimodal NMR Analysis. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 6443-6449	6.4	12
66	Adsorption and Thermal Decomposition of Electrolytes on Nanometer Magnesium Oxide: An in Situ C MAS NMR Study. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 38689-38696	9.5	12
65	The formation of Gluconacetobacter xylinum cellulose under the influence of the dye brilliant yellow. <i>Cellulose</i> , 2019 , 26, 9373-9386	5.5	1
64	A multi-functional interface derived from thiol-modified mesoporous carbon in lithium-sulfur batteries. <i>Journal of Materials Chemistry A</i> , 2019 , 7, 13372-13381	13	11
63	Evolution of Ion-Ion Interactions and Structures in Smectic Ionic Liquid Crystals. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 20547-20557	3.8	6
62	Role of Inorganic Surface Layer on Solid Electrolyte Interphase Evolution at Li-Metal Anodes. <i>ACS Applied Materials & Interfaces</i> , 2019 , 11, 31467-31476	9.5	47
61	Mechanism by which Tungsten Oxide Promotes the Activity of Supported V ₂ O ₅ /TiO ₂ Catalysts for NO Abatement: Structural Effects Revealed by V MAS NMR Spectroscopy. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 12609-12616	16.4	48
60	Mechanism by which Tungsten Oxide Promotes the Activity of Supported V ₂ O ₅ /TiO ₂ Catalysts for NO _x Abatement: Structural Effects Revealed by 51V MAS NMR Spectroscopy. <i>Angewandte Chemie</i> , 2019 , 131, 12739-12746	3.6	30
59	Monitoring solvent dynamics and ion associations in the formation of cubic octamer polyanion in tetramethylammonium silicate solutions. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 4717-4720	3.6	4
58	Structure and Dynamics of Polysulfide Clusters in a Nonaqueous Solvent Mixture of 1,3-Dioxolane and 1,2-Dimethoxyethane. <i>Chemistry of Materials</i> , 2019 , 31, 2308-2319	9.6	36
57	Addressing Passivation in Lithium-Sulfur Battery Under Lean Electrolyte Condition. <i>Advanced Functional Materials</i> , 2018 , 28, 1707234	15.6	111
56	In situ and ex situ NMR for battery research. <i>Journal of Physics Condensed Matter</i> , 2018 , 30, 463001	1.8	22
55	Lean Electrolyte Batteries: Addressing Passivation in Lithium-Sulfur Battery Under Lean Electrolyte Condition (Adv. Funct. Mater. 38/2018). <i>Advanced Functional Materials</i> , 2018 , 28, 1870275	15.6	5
54	Calculations of solid-state Ca NMR parameters: A comparison of periodic and cluster approaches and an evaluation of DFT functionals. <i>Journal of Computational Chemistry</i> , 2017 , 38, 949-956	3.5	18
53	Surface Interactions and Confinement of Methane: A High Pressure Magic Angle Spinning NMR and Computational Chemistry Study. <i>Langmuir</i> , 2017 , 33, 1359-1367	4	16
52	Semi-empirical refinements of crystal structures using O quadrupolar-coupling tensors. <i>Journal of Chemical Physics</i> , 2017 , 146, 064201	3.9	18
51	In Situ Chemical Imaging of Solid-Electrolyte Interphase Layer Evolution in Li-S Batteries. <i>Chemistry of Materials</i> , 2017 , 29, 4728-4737	9.6	98

50	Improving Lithium-Sulfur Battery Performance under Lean Electrolyte through Nanoscale Confinement in Soft Swellable Gels. <i>Nano Letters</i> , 2017 , 17, 3061-3067	11.5	99
49	Toward high-resolution NMR spectroscopy of microscopic liquid samples. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 14256-14261	3.6	4
48	Multinuclear NMR Study of the Solid Electrolyte Interface Formed in Lithium Metal Batteries. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 14741-14748	9.5	36
47	Elucidating the Solvation Structure and Dynamics of Lithium Polysulfides Resulting from Competitive Salt and Solvent Interactions. <i>Chemistry of Materials</i> , 2017 , 29, 3375-3379	9.6	78
46	Ammonium Additives to Dissolve Lithium Sulfide through Hydrogen Binding for High-Energy Lithium-Sulfur Batteries. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 4290-4295	9.5	51
45	Imaging Electrochemical Processes in Li Batteries by Operando STEM. <i>Microscopy and Microanalysis</i> , 2017 , 23, 1970-1971	0.5	1
44	Fabrication of phosphonic acid films on nitinol nanoparticles by dynamic covalent assembly. <i>Thin Solid Films</i> , 2017 , 642, 195-206	2.2	8
43	Controlling Solid-Liquid Conversion Reactions for a Highly Reversible Aqueous Zinc-Battery. <i>ACS Energy Letters</i> , 2017 , 2, 2674-2680	20.1	96
42	High-resolution microstrip NMR detectors for subnanoliter samples. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 28163-28174	3.6	8
41	Non-encapsulation approach for high-performance LiS batteries through controlled nucleation and growth. <i>Nature Energy</i> , 2017 , 2, 813-820	62.3	256
40	Effects of Anion Mobility on Electrochemical Behaviors of Lithium-Sulfur Batteries. <i>Chemistry of Materials</i> , 2017 , 29, 9023-9029	9.6	28
39	Uranium Release from Acidic Weathered Hanford Sediments: Single-Pass Flow-Through and Column Experiments. <i>Environmental Science & Technology</i> , 2017 , 51, 11011-11019	10.3	11
38	Study of Perfluorophosphonic Acid Surface Modifications on Zinc Oxide Nanoparticles. <i>Materials</i> , 2017 , 10,	3.5	17
37	Reversible aqueous zinc/manganese oxide energy storage from conversion reactions. <i>Nature Energy</i> , 2016 , 1,	62.3	1461
36	Preferential Solvation of an Asymmetric Redox Molecule. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 27834-27839	3.6	11
35	Liquid Crystals: Facilitated Ion Transport in Smectic Ordered Ionic Liquid Crystals (Adv. Mater. 42/2016). <i>Advanced Materials</i> , 2016 , 28, 9439-9439	24	1
34	The Impact of Li Grain Size on Coulombic Efficiency in Li Batteries. <i>Scientific Reports</i> , 2016 , 6, 34267	4.9	53
33	Understanding the Effect of Additives in Li-ion and Li-Sulfur Batteries by Operando ec- (S)TEM. <i>Microscopy and Microanalysis</i> , 2016 , 22, 22-23	0.5	5

32	Nuclear magnetic resonance studies of the solvation structures of a high-performance nonaqueous redox flow electrolyte. <i>Journal of Power Sources</i> , 2016 , 308, 172-179	8.9	15
31	Sustainable development of a surface-functionalized mesoporous aluminosilicate with ultra-high ion exchange efficiency. <i>Inorganic Chemistry Frontiers</i> , 2016 , 3, 502-513	6.8	17
30	Molecular Storage of Mg Ions with Vanadium Oxide Nanoclusters. <i>Advanced Functional Materials</i> , 2016 , 26, 3446-3453	15.6	50
29	Restricting the Solubility of Polysulfides in Li-S Batteries Via Electrolyte Salt Selection. <i>Advanced Energy Materials</i> , 2016 , 6, 1600160	21.8	57
28	Analysis of the bond-valence method for calculating (29) Si and (31) P magnetic shielding in covalent network solids. <i>Journal of Computational Chemistry</i> , 2016 , 37, 1704-10	3.5	13
27	Effect of the Anion Activity on the Stability of Li Metal Anodes in Lithium-Sulfur Batteries. <i>Advanced Functional Materials</i> , 2016 , 26, 3059-3066	15.6	89
26	Diffusive Flux as a New Metric for Ion-Conducting Soft Materials. <i>ACS Energy Letters</i> , 2016 , 1, 1179-1183	20.1	11
25	The diffusion and conduction of lithium in poly(ethylene oxide)-based sulfonate ionomers. <i>Journal of Chemical Physics</i> , 2016 , 145, 114903	3.9	12
24	Facilitated Ion Transport in Smectic Ordered Ionic Liquid Crystals. <i>Advanced Materials</i> , 2016 , 28, 9301-9307	17	29
23	Critical Analysis of Cluster Models and Exchange-Correlation Functionals for Calculating Magnetic Shielding in Molecular Solids. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5229-41	6.4	49
22	Solvation structure and transport properties of alkali cations in dimethyl sulfoxide under exogenous static electric fields. <i>Journal of Chemical Physics</i> , 2015 , 142, 224502	3.9	8
21	Experiences with a researcher-centric ELN. <i>Chemical Science</i> , 2015 , 6, 1614-1629	9.4	18
20	Monitoring the refinement of crystal structures with (15)N solid-state NMR shift tensor data. <i>Journal of Chemical Physics</i> , 2015 , 143, 194702	3.9	26
19	Nanocomposite polymer electrolyte for rechargeable magnesium batteries. <i>Nano Energy</i> , 2015 , 12, 750-759	17.9	86
18	Density functional investigation of intermolecular effects on 13C NMR chemical-shielding tensors modeled with molecular clusters. <i>Journal of Chemical Physics</i> , 2014 , 141, 164121	3.9	47
17	Diffusional motion of redox centers in carbonate electrolytes. <i>Journal of Chemical Physics</i> , 2014 , 141, 104509	3.9	21
16	Solid state nuclear magnetic resonance investigation of polymer backbone dynamics in poly(ethylene oxide) based lithium and sodium polyether-ester-sulfonate ionomers. <i>Journal of Chemical Physics</i> , 2013 , 138, 194907	3.9	8
15	Nuclear magnetic resonance investigation of dynamics in poly(ethylene oxide)-based lithium polyether-ester-sulfonate ionomers. <i>Journal of Chemical Physics</i> , 2012 , 136, 014510	3.9	20

14	Effect of SiO ₂ on Densification and Microstructure Development in Nd:YAG Transparent Ceramics. <i>Journal of the American Ceramic Society</i> , 2011 , 94, 1380-1387	3.8	113
13	Cesium and strontium incorporation into zeolite-type phases during homogeneous nucleation from caustic solutions. <i>American Mineralogist</i> , 2011 , 96, 1809-1820	2.9	8
12	Description of Mg ²⁺ Release from Forsterite Using Ab Initio Methods <i>Journal of Physical Chemistry C</i> , 2010 , 114, 5417-5428	3.8	15
11	Characterization of cation environments in polycrystalline forsterite by 25Mg MAS, MQMAS, and QCPMG NMR. <i>American Mineralogist</i> , 2010 , 95, 1601-1607	2.9	10
10	Computational Spectroscopy in Environmental Chemistry 2010 , 323-351		2
9	Intermolecular shielding contributions studied by modeling the (13)C chemical-shift tensors of organic single crystals with plane waves. <i>Journal of Chemical Physics</i> , 2009 , 131, 144503	3.9	71
8	Silicon control of strontium and cesium partitioning in hydroxide-weathered sediments. <i>Geochimica Et Cosmochimica Acta</i> , 2008 , 72, 2024-2047	5.5	48
7	Investigation of Lead Borosilicate Glass Structure With 207Pb and 11B Solid-State NMR. <i>Materials Research Society Symposia Proceedings</i> , 2000 , 658, 3221		
6	Determination of internuclear distances from solid-state nuclear magnetic resonance: Dipolar transforms and regularization methods. <i>Molecular Physics</i> , 1998 , 95, 907-919	1.7	20
5	Synthesis of Porous Transition Metal Oxides by the Salt-Gel Method. <i>Materials Research Society Symposia Proceedings</i> , 1994 , 371, 69		5
4	High-resolution oxygen-17 NMR of solid silicates. <i>Journal of the American Chemical Society</i> , 1991 , 113, 32-38	16.4	104
3	Dynamic-angle spinning of quadrupolar nuclei. <i>Journal of Magnetic Resonance</i> , 1990 , 86, 470-487		58
2	Determination of internuclear distances from solid-state nuclear magnetic resonance: Dipolar transforms and regularization methods		3
1	Solvation Structure and Dynamics of Mg(TFSI) ₂ Aqueous Electrolyte. <i>Energy and Environmental Materials</i> ,	13	6