Andrew J Pell

List of Publications by Year
in descending order

63 papers	3,496 citations	159585 30 h-index	138484 58 g-index
67 all docs	67 docs citations	67 times ranked	4299 citing authors

#	Article	IF	Citations
1	Identifying the Critical Role of Li Substitution in P2â€“Na_x[Li_yNi_zMn_{1â€“yâ€“z}]O₂ (0 < x, y, z < 1) Intercalation Cathode Materials for High-Energy Na-Ion Batteries. Chemistry of Materials, 2014, 26, 1260-1269.	6.7	417
2	Paramagnetic NMR in solution and the solid state. Progress in Nuclear Magnetic Resonance Spectroscopy, 2019, 111, 1-271.	7.5	274
3	Rapid Proton-Detected NMR Assignment for Proteins with Fast Magic Angle Spinning. Journal of the American Chemical Society, 2014, 136, 12489-12497.	13.7	254
4	Local Environments of Dilute Activator Ions in the Solid-State Lighting Phosphor Y_{3â€“x}Ce_xAl₅O₁₂. Chemistry of Materials, 2013, 25, 3979-3995.	6.7	208
5	Solid Electrolyte Interphase Growth and Capacity Loss in Silicon Electrodes. Journal of the American Chemical Society, 2016, 138, 7918-7931.	13.7	189
6	Structure and backbone dynamics of a microcrystalline metalloprotein by solid-state NMR. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 11095-11100.	7.1	173
7	Fast Resonance Assignment and Fold Determination of Human Superoxide Dismutase by Highâ€Resolution Protonâ€Detected Solidâ€State MAS NMR Spectroscopy. Angewandte Chemie - International Edition, 2011, 50, 11697-11701.	13.8	157
8	Two-dimensional J-spectra with absorption-mode lineshapes. Journal of Magnetic Resonance, 2007, 189, 293-299.	2.1	126
9	Spin-Transfer Pathways in Paramagnetic Lithium Transition-Metal Phosphates from Combined Broadband Isotropic Solid-State MAS NMR Spectroscopy and DFT Calculations. Journal of the American Chemical Society, 2012, 134, 17178-17185.	13.7	122
10	Broadband proton-decoupled proton spectra. Magnetic Resonance in Chemistry, 2007, 45, 296-316.	1.9	114
11	Cellulose from the green macroalgae Ulva lactuca: isolation, characterization, optotracing, and production of cellulose nanofibrils. Cellulose, 2020, 27, 3707-3725.	4.9	91
12	Selective Control of Composition in Prussian White for Enhanced Material Properties. Chemistry of Materials, 2019, 31, 7203-7211.	6.7	86
13	Characterizing Oxygen Local Environments in Paramagnetic Battery Materials via ¹⁷O NMR and DFT Calculations. Journal of the American Chemical Society, 2016, 138, 9405-9408.	13.7	74
14	Correlating Local Compositions and Structures with the Macroscopic Optical Properties of Ce³⁺-Doped CaSc₂O₄, an Efficient Green-Emitting Phosphor. Chemistry of Materials, 2017, 29, 3538-3546.	6.7	66
15	Exfoliation of Layered Na-Ion Anode Material Na₂Ti₃O₇ for Enhanced Capacity and Cyclability. Chemistry of Materials, 2018, 30, 1505-1516.	6.7	63
16	Dynamic Nuclear Polarizationâ€Enhanced Biomolecular NMR Spectroscopy at High Magnetic Field with Fast Magicâ€Angle Spinning. Angewandte Chemie - International Edition, 2018, 57, 7458-7462.	13.8	56
17	Out-and-back 13Câ€“13C scalar transfers in protein resonance assignment by proton-detected solid-state NMR under ultra-fast MAS. Journal of Biomolecular NMR, 2013, 56, 379-386.	2.8	54
18	Broadband solid-state MAS NMR of paramagnetic systems. Progress in Nuclear Magnetic Resonance Spectroscopy, 2015, 84-85, 33-72.	7.5	54

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19	¹H-Detected Biomolecular NMR under Fast Magic-Angle Spinning. Chemical Reviews, 2022, 122, 9943-10018.	47.7	51
20	Characterising local environments in high energy density Li-ion battery cathodes: a combined NMR and first principles study of LiFe_xCo_{1â^'x}PO₄. Journal of Materials Chemistry A, 2014, 2, 11948-11957.	10.3	50
21	A systematic study of ²⁵Mg NMR in paramagnetic transition metal oxides: applications to Mg-ion battery materials. Physical Chemistry Chemical Physics, 2017, 19, 613-625.	2.8	50
22	Broadband inversion for MAS NMR with single-sideband-selective adiabatic pulses. Journal of Chemical Physics, 2011, 134, 024117.	3.0	41
23	Frequency-stepped acquisition in nuclear magnetic resonance spectroscopy under magic angle spinning. Journal of Chemical Physics, 2013, 138, 114201.	3.0	40
24	Observing an Antisense Drug Complex in Intact Human Cells by inâ€Cell NMR Spectroscopy. ChemBioChem, 2019, 20, 2474-2478.	2.6	38
25	Large-Scale Computation of Nuclear Magnetic Resonance Shifts for Paramagnetic Solids Using CP2K. Journal of Chemical Theory and Computation, 2018, 14, 377-394.	5.3	34
26	Nature of Chemisorbed CO₂ in Zeolite A. Journal of Physical Chemistry C, 2019, 123, 21497-21503.	3.1	34
27	Picometer Resolution Structure of the Coordination Sphere in the Metal-Binding Site in a Metalloprotein by NMR. Journal of the American Chemical Society, 2020, 142, 16757-16765.	13.7	33
28	Residual Lignin and Zwitterionic Polymer Grafts on Cellulose Nanocrystals for Antifouling and Antibacterial Applications. ACS Applied Polymer Materials, 2020, 2, 3060-3071.	4.4	32
29	DFT investigation of the effect of spin-orbit coupling on the NMR shifts in paramagnetic solids. Physical Review B, 2017, 95, .	3.2	31
30	Polymorphism and magnetic properties of Li2MSiO4 (M = Fe, Mn) cathode materials. Scientific Reports, 2013, 3, 3452.	3.3	29
31	Exploring the Origins of Improved Photocurrent by Acidic Treatment for Quaternary Tantalum-Based Oxynitride Photoanodes on the Example of CaTaO₂N. Journal of Physical Chemistry C, 2020, 124, 152-160.	3.1	28
32	Electrochemical Denitrification and Oxidative Dehydrogenation of Ethylbenzene over N-doped Mesoporous Carbon: Atomic Level Understanding of Catalytic Activity by ¹⁵N NMR Spectroscopy. Chemistry of Materials, 2020, 32, 7263-7273.	6.7	28
33	Structural Characterization of the Li-Ion Battery Cathode Materials LiTi_xMn_{2â€“x}O₄ (0.2 â‰¤ x â‰¤ 1.5): A Combined Experimental ⁷Li NMR and First-Principles Study. Chemistry of Materials, 2018, 30, 817-829.	6.7	27
34	Hydride Reduction of BaTiO₃ â^' Oxyhydride Versus O Vacancy Formation. ACS Omega, 2018, 3, 11426-11438.	3.5	27
35	Low-power broadband solid-state MAS NMR of 14N. Journal of Chemical Physics, 2017, 146, 194202.	3.0	26
36	When Do Anisotropic Magnetic Susceptibilities Lead to Large NMR Shifts? Exploring Particle Shape Effects in the Battery Electrode Material LiFePO₄. Journal of the American Chemical Society, 2019, 141, 13089-13100.	13.7	22

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37	Combination of DQ and ZQ Coherences for Sensitive Throughâ€Bond NMR Correlation Experiments in Biosolids under Ultraâ€Fast MAS. ChemPhysChem, 2012, 13, 2405-2411.	2.1	21
38	¹³Câ€Detected Throughâ€Bond Correlation Experiments for Protein Resonance Assignment by Ultraâ€Fast MAS Solidâ€State NMR. ChemPhysChem, 2013, 14, 3131-3137.	2.1	19
39	Dynamics of Hydride Ions in Metal Hydride-Reduced BaTiO₃ Samples Investigated with Quasielastic Neutron Scattering. Journal of Physical Chemistry C, 2019, 123, 2019-2030.	3.1	19
40	Crystal and electronic facet analysis of ultrafine Ni2P particles by solid-state NMR nanocrystallography. Nature Communications, 2021, 12, 4334.	12.8	17
41	Single crystal nuclear magnetic resonance in spinning powders. Journal of Chemical Physics, 2011, 135, 144201.	3.0	14
42	Ni₂P Nanoparticles Embedded in Mesoporous SiO₂ for Catalytic Hydrogenation of SO₂ to Elemental S. ACS Applied Nano Materials, 2021, 4, 5665-5676.	5.0	14
43	Resolving Dirac electrons with broadband high-resolution NMR. Nature Communications, 2020, 11, 1285.	12.8	13
44	Insights into the Exfoliation Process of V₂O₅Â·nH₂O Nanosheet Formation Using Real-Time ⁵¹V NMR. ACS Omega, 2019, 4, 10899-10905.	3.5	12
45	Synthesis and Physical Properties of the Oxofluoride Cu2(SeO3)F2. Inorganic Chemistry, 2018, 57, 4640-4648.	4.0	11
46	Nickel Phosphide Nanoparticles for Selective Hydrogenation of SO₂ to H₂S. ACS Applied Nano Materials, 2021, 4, 6568-6582.	5.0	11
47	Melilite LaSrGa_{3â^'x}Al_xO₇ Series: A Combined Solid-State NMR and Neutron Diffraction Study. Journal of Physical Chemistry C, 2014, 118, 15036-15043.	3.1	10
48	Broadband MAS NMR spectroscopy in the low-power limit. Chemical Physics Letters, 2018, 697, 29-37.	2.6	10
49	Mysterious SiB₃: Identifying the Relation between Î±- and Î²-SiB₃. ACS Omega, 2019, 4, 18741-18759.	3.5	9
50	The role of oxygen vacancies on the vibrational motions of hydride ions in the oxyhydride of barium titanate. Journal of Materials Chemistry A, 2020, 8, 6360-6371.	10.3	9
51	Dynamic Nuclear Polarizationâ€Enhanced Biomolecular NMR Spectroscopy at High Magnetic Field with Fast Magicâ€Angle Spinning. Angewandte Chemie, 2018, 130, 7580-7584.	2.0	8
52	Artefact-free broadband 2D NMR for separation of quadrupolar and paramagnetic shift interactions. Solid State Nuclear Magnetic Resonance, 2019, 101, 51-62.	2.3	8
53	A biocompatible ZnNa2-based metalâ€“organic framework with high ibuprofen, nitric oxide and metal uptake capacity. Materials Advances, 2020, 1, 2248-2260.	5.4	8
54	Frequency-swept adiabatic pulses for broadband solid-state MAS NMR. Journal of Magnetic Resonance, 2021, 324, 106911.	2.1	8

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55	A method to calculate the NMR spectra of paramagnetic species using thermalized electronic relaxation. Journal of Magnetic Resonance, 2021, 326, 106939.	2.1	8
56	Investigation of the Orderâ€“Disorder Rotator Phase Transition in KSiH₃ and RbSiH₃. Journal of Physical Chemistry C, 2017, 121, 5241-5252.	3.1	6
57	Low-power synchronous helical pulse sequences for large anisotropic interactions in MAS NMR: Double-quantum excitation of 14N. Journal of Chemical Physics, 2020, 153, 244202.	3.0	6
58	Separation of quadrupolar and paramagnetic shift interactions with TOPâ€STMAS/MQMAS in solidâ€state lighting phosphors. Magnetic Resonance in Chemistry, 2020, 58, 1055-1070.	1.9	6
59	Indium(III) in the â€œPeriodic Tableâ€•of Di(2-pyridyl) Ketone: An Unprecedented Transformation of the Ligand and Solid-State 115In NMR Spectroscopy as a Valuable Structural Tool. Inorganic Chemistry, 2021, 60, 4829-4840.	4.0	4
60	Computational insight into the hydrogenation of CO2 and carbamic acids to methanol by a ruthenium(II)-based catalyst: The role of amino (NH) ligand group. Molecular Catalysis, 2021, 506, 111544.	2.0	4
61	Separation of quadrupolar and paramagnetic shift interactions in high-resolution nuclear magnetic resonance of spinning powders. Journal of Chemical Physics, 2021, 155, 094202.	3.0	4
62	Proton-detected fast-magic-angle spinning NMR of paramagnetic inorganic solids. RSC Advances, 2021, 11, 29870-29876.	3.6	3
63	Half-integer-spin quadrupolar nuclei in magic-angle spinning paramagnetic NMR: The case of NaMnO2. Journal of Magnetic Resonance, 2022, , 107235.	2.1	2