List of Publications by Year in descending order

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DAVID CALAN

#	Article	IF	CITATIONS
1	Harnessing Catalysis Selectivity and Isophorone Diisocyanate Asymmetry for Tailored Polyurethane Prepolymers and Networks. Macromolecules, 2022, 55, 3344-3352.	4.8	5
2	Multiple Surface Site Three-Dimensional Structure Determination of a Supported Molecular Catalyst. Journal of the American Chemical Society, 2022, 144, 10270-10281.	13.7	9
3	Atomic-Scale Structure and Its Impact on Chemical Properties of Aluminum Oxide Layers Prepared by Atomic Layer Deposition on Silica. Chemistry of Materials, 2021, 33, 3335-3348.	6.7	23
4	Spectroscopic Signature and Structure of the Active Sites in Ziegler–Natta Polymerization Catalysts Revealed by Electron Paramagnetic Resonance. Journal of the American Chemical Society, 2021, 143, 9791-9797.	13.7	19
5	Ni(<scp>ii</scp>) and Co(<scp>ii</scp>) bis(acetylacetonato) complexes for alkene/vinylsilane silylation and silicone crosslinking. Catalysis Science and Technology, 2021, 11, 4849-4856.	4.1	1
6	Toward the Coordination Fingerprint of the Edge-Sharing BO ₄ Tetrahedra. Inorganic Chemistry, 2021, 60, 2406-2413.	4.0	6
7	Efficient Dynamic Nuclear Polarization up to 230 K with Hybrid BDPA-Nitroxide Radicals at a High Magnetic Field. Journal of Physical Chemistry B, 2021, 125, 13329-13338.	2.6	9
8	Stepwise construction of silica-supported tantalum/iridium heteropolymetallic catalysts using surface organometallic chemistry. Journal of Catalysis, 2020, 392, 287-301.	6.2	11
9	The Structure of Molecular and Surface Platinum Sites Determined by DNP-SENS and Fast MAS ¹⁹⁵ Pt Solid-State NMR Spectroscopy. Journal of the American Chemical Society, 2020, 142, 18936-18945.	13.7	35
10	Atomicâ€Scale Description of Interfaces between Antigen and Aluminumâ€Based Adjuvants Used in Vaccines by Dynamic Nuclear Polarization (DNP) Enhanced NMR Spectroscopy. Chemistry - A European Journal, 2020, 26, 8976-8982.	3.3	13
11	One-pot syntheses of heterotelechelic α-vinyl,ï‰-methoxysilane polyethylenes and condensation into comb-like and star-like polymers with high chain end functionality. Polymer Chemistry, 2020, 11, 3884-3891.	3.9	11
12	TinyPols: a family of water-soluble binitroxides tailored for dynamic nuclear polarization enhanced NMR spectroscopy at 18.8 and 21.1 T. Chemical Science, 2020, 11, 2810-2818.	7.4	72
13	Specific Localization of Aluminum Sites Favors Ethene-to-Propene Conversion on (Al)MCM-41-Supported Ni(II) Single Sites. ACS Catalysis, 2019, 9, 7476-7485.	11.2	24
14	Metal–Metal Synergy in Well-Defined Surface Tantalum–Iridium Heterobimetallic Catalysts for H/D Exchange Reactions. Journal of the American Chemical Society, 2019, 141, 19321-19335.	13.7	33
15	Beyond Î ³ -Al2O3 crystallite surfaces: The hidden features of edges revealed by solid-state 1H NMR and DFT calculations. Journal of Catalysis, 2019, 378, 140-143.	6.2	36
16	Supported Ru olefin metathesis catalysts <i>via</i> a thiolate tether. Dalton Transactions, 2019, 48, 2886-2890.	3.3	5
17	19 F Magic Angle Spinning Dynamic Nuclear Polarization Enhanced NMR Spectroscopy. Angewandte Chemie, 2019, 131, 7327-7331.	2.0	2
18	Structural description of surfaces and interfaces in biominerals by DNP SENS. Solid State Nuclear Magnetic Resonance, 2019, 102, 2-11.	2.3	25

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19	Aromatic Ring Dynamics, Thermal Activation, and Transient Conformations of a 468 kDa Enzyme by Specific ¹ H– ¹³ C Labeling and Fast Magic-Angle Spinning NMR. Journal of the American Chemical Society, 2019, 141, 11183-11195.	13.7	43
20	Innenrücktitelbild: Preferential Siting of Aluminum Heteroatoms in the Zeolite Catalyst Al‧SZâ€70 (Angew. Chem. 19/2019). Angewandte Chemie, 2019, 131, 6523-6523.	2.0	0
21	Preferential Siting of Aluminum Heteroatoms in the Zeolite Catalyst Alâ€SSZâ€70. Angewandte Chemie - International Edition, 2019, 58, 6255-6259.	13.8	31
22	Preferential Siting of Aluminum Heteroatoms in the Zeolite Catalyst Al SZâ€70. Angewandte Chemie, 2019, 131, 6321-6325.	2.0	10
23	¹⁹ F Magic Angle Spinning Dynamic Nuclear Polarization Enhanced NMR Spectroscopy. Angewandte Chemie - International Edition, 2019, 58, 7249-7253.	13.8	18
24	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
25	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
26	Predicting the DNP-SENS efficiency in reactive heterogeneous catalysts from hydrophilicity. Chemical Science, 2018, 9, 4866-4872.	7.4	24
27	BDPA-Nitroxide Biradicals Tailored for Efficient Dynamic Nuclear Polarization Enhanced Solid-State NMR at Magnetic Fields up to 21.1 T. Journal of the American Chemical Society, 2018, 140, 13340-13349.	13.7	99
28	Transportable hyperpolarized metabolites. Nature Communications, 2017, 8, 13975.	12.8	86
29	Oxygen-17 dynamic nuclear polarisation enhanced solid-state NMR spectroscopy at 18.8 T. Chemical Communications, 2017, 53, 2563-2566.	4.1	39
30	Tailored Polarizing Hybrid Solids with Nitroxide Radicals Localized in Mesostructured Silica Walls. Helvetica Chimica Acta, 2017, 100, e1700101.	1.6	24
31	Frozen Acrylamide Gels as Dynamic Nuclear Polarization Matrices. Angewandte Chemie - International Edition, 2017, 56, 8726-8730.	13.8	26
32	From single-site tantalum complexes to nanoparticles of Ta _x N _y and TaO _x N _y supported on silica: elucidation of synthesis chemistry by dynamic nuclear polarization surface enhanced NMR spectroscopy and X-ray absorption spectroscopy. Chemical Science, 2017, 8, 5650-5661.	7.4	14
33	The structure and binding mode of citrate in the stabilization of gold nanoparticles. Nature Chemistry, 2017, 9, 890-895.	13.6	222
34	Phenylazide Hybridâ€ s ilica – Polarization Platform for Dynamic Nuclear Polarization at Cryogenic Temperatures. Helvetica Chimica Acta, 2017, 100, e1600122.	1.6	6
35	Three-Dimensional Structure Determination of Surface Sites. Journal of the American Chemical Society, 2017, 139, 849-855.	13.7	75
36	Frozen Acrylamide Gels as Dynamic Nuclear Polarization Matrices. Angewandte Chemie, 2017, 129, 8852-8856.	2.0	2

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37	Dynamic Nuclear Polarization Efficiency Increased by Very Fast Magic Angle Spinning. Journal of the American Chemical Society, 2017, 139, 10609-10612.	13.7	52
38	Reactive surface organometallic complexes observed using dynamic nuclear polarization surface enhanced NMR spectroscopy. Chemical Science, 2017, 8, 284-290.	7.4	55
39	Dendritic polarizing agents for DNP SENS. Chemical Science, 2017, 8, 416-422.	7.4	35
40	Atomistic Description of Reaction Intermediates for Supported Metathesis Catalysts Enabled by DNP SENS. Angewandte Chemie, 2016, 128, 4821-4825.	2.0	6
41	Hyperpolarization of Frozen Hydrocarbon Gases by Dynamic Nuclear Polarization at 1.2 K. Journal of Physical Chemistry Letters, 2016, 7, 3235-3239.	4.6	18
42	Cubic three-dimensional hybrid silica solids for nuclear hyperpolarization. Chemical Science, 2016, 7, 6846-6850.	7.4	19
43	Structural Characterization of the EtOH–TiCl ₄ –MgCl ₂ Ziegler–Natta Precatalyst. Journal of Physical Chemistry C, 2016, 120, 18075-18087.	3.1	28
44	Atomistic Description of Reaction Intermediates for Supported Metathesis Catalysts Enabled by DNP SENS. Angewandte Chemie - International Edition, 2016, 55, 4743-4747.	13.8	52
45	Atomic-level organization of vicinal acid–base pairs through the chemisorption of aniline and derivatives onto mesoporous SBA15. Chemical Science, 2016, 7, 6099-6105.	7.4	16
46	Predictive morphology, stoichiometry and structure of surface species in supported Ru nanoparticles under H ₂ and CO atmospheres from combined experimental and DFT studies. Physical Chemistry Chemical Physics, 2016, 18, 1969-1979.	2.8	36
47	Dynamic nuclear polarization at 40 kHz magic angle spinning. Physical Chemistry Chemical Physics, 2016, 18, 10616-10622.	2.8	74
48	The Nature of Secondary Interactions at Electrophilic Metal Sites of Molecular and Silica-Supported Organolutetium Complexes from Solid-State NMR Spectroscopy. Journal of the American Chemical Society, 2016, 138, 3831-3843.	13.7	35
49	Iridium(I)/Nâ€Heterocyclic Carbene Hybrid Materials: Surface Stabilization of Lowâ€Valent Iridium Species for High Catalytic Hydrogenation Performance. Angewandte Chemie - International Edition, 2015, 54, 12937-12941.	13.8	33
50	Solid-State Dynamic Nuclear Polarization at 9.4 and 18.8 T from 100 K to Room Temperature. Journal of the American Chemical Society, 2015, 137, 14558-14561.	13.7	87
51	Influences of Dilute Organic Adsorbates on the Hydration of Low-Surface-Area Silicates. Journal of the American Chemical Society, 2015, 137, 8096-8112.	13.7	85
52	Polymorphs of Theophylline Characterized by DNP Enhanced Solid-State NMR. Molecular Pharmaceutics, 2015, 12, 4146-4153.	4.6	77
53	Hybrid polarizing solids for pure hyperpolarized liquids through dissolution dynamic nuclear polarization. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 14693-14697.	7.1	93
54	A Wellâ€Defined Pd Hybrid Material for the <i>Z</i> â€Selective Semihydrogenation of Alkynes Characterized at the Molecular Level by DNP SENS. Chemistry - A European Journal, 2013, 19, 12234-12238.	3.3	61

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55	A Well-Defined Silica-Supported Tungsten Oxo Alkylidene Is a Highly Active Alkene Metathesis Catalyst. Journal of the American Chemical Society, 2013, 135, 19068-19070.	13.7	83
56	Solid-Phase Polarization Matrixes for Dynamic Nuclear Polarization from Homogeneously Distributed Radicals in Mesostructured Hybrid Silica Materials. Journal of the American Chemical Society, 2013, 135, 15459-15466.	13.7	56
57	Molecular-level characterization of the structure and the surface chemistry of periodic mesoporous organosilicates using DNP-surface enhanced NMR spectroscopy. Physical Chemistry Chemical Physics, 2013, 15, 13270.	2.8	56
58	Evidence for Metal–Surface Interactions and Their Role in Stabilizing Well-Defined Immobilized Ru–NHC Alkene Metathesis Catalysts. Journal of the American Chemical Society, 2013, 135, 3193-3199.	13.7	96
59	A Slowly Relaxing Rigid Biradical for Efficient Dynamic Nuclear Polarization Surface-Enhanced NMR Spectroscopy: Expeditious Characterization of Functional Group Manipulation in Hybrid Materials. Journal of the American Chemical Society, 2012, 134, 2284-2291.	13.7	182
60	Dynamic Nuclear Polarization NMR Spectroscopy of Microcrystalline Solids. Journal of the American Chemical Society, 2012, 134, 16899-16908.	13.7	242
61	Dynamic nuclear polarization of quadrupolar nuclei using cross polarization from protons: surface-enhanced aluminium-27 NMR. Chemical Communications, 2012, 48, 1988.	4.1	123
62	Non-aqueous solvents for DNP surface enhanced NMR spectroscopy. Chemical Communications, 2012, 48, 654-656.	4.1	155
63	One hundred fold overall sensitivity enhancements for Silicon-29 NMR spectroscopy of surfaces by dynamic nuclear polarization with CPMG acquisition. Chemical Science, 2012, 3, 108-115.	7.4	141
64	Solid-state NMR: a key tool for the understanding at a molecular level of well-defined heterogeneous catalysts and surface chemistry on top of oxide materials. Spectroscopic Properties of Inorganic and Organometallic Compounds, 2012, , 57-83.	0.4	2
65	Silica-supported single-site catalysts: to be or not to be? A conjecture on silica surfaces. New Journal of Chemistry, 2011, 35, 2403.	2.8	70
66	Probing surface site heterogeneity through 1D and INADEQUATE 31P solid state NMR spectroscopy of silica supported PMe3-Au(I) adducts. Chemical Science, 2011, 2, 928.	7.4	15
67	Fast Characterization of Functionalized Silica Materials by Silicon-29 Surface-Enhanced NMR Spectroscopy Using Dynamic Nuclear Polarization. Journal of the American Chemical Society, 2011, 133, 2104-2107.	13.7	254
68	A highly ordered mesostructured material containing regularly distributed phenols: preparation and characterization at a molecular level through ultra-fast magic angle spinning proton NMR spectroscopy. Physical Chemistry Chemical Physics, 2011, 13, 4230.	2.8	13
69	Surface Enhanced NMR Spectroscopy by Dynamic Nuclear Polarization. Journal of the American Chemical Society, 2010, 132, 15459-15461.	13.7	488
70	Synthesis and reactivity of molybdenum imido alkylidene bis-pyrazolide complexes. Dalton Transactions, 2010, 39, 8547.	3.3	18
71	Wellâ€Defined Silica‧upported Mo–Alkylidene Catalyst Precursors Containing One OR Substituent: Methods of Preparation and Structure–Reactivity Relationship in Alkene Metathesis. Chemistry - A European Journal, 2009, 15, 5083-5089.	3.3	53
72	Gold Nanoparticles Supported on Passivated Silica: Access to an Efficient Aerobic Epoxidation Catalyst and the Intrinsic Oxidation Activity of Gold. Journal of the American Chemical Society, 2009, 131, 14667-14669.	13.7	111

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73	Hydrogen and oxygen adsorption stoichiometries on silica supported ruthenium nanoparticles. Journal of Catalysis, 2008, 260, 387-391.	6.2	35