

# Frédéric A Perras

## List of Publications by Year in descending order

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81  
papers

3,029  
citations

147801

31  
h-index

168389

53  
g-index

87  
all docs

87  
docs citations

87  
times ranked

2902  
citing authors

#	ARTICLE	IF	CITATIONS
1	Upcycling Single-Use Polyethylene into High-Quality Liquid Products. ACS Central Science, 2019, 5, 1795-1803.	11.3	283
2	Catalytic upcycling of high-density polyethylene via a processive mechanism. Nature Catalysis, 2020, 3, 893-901.	34.4	262
3	Dynamic Nuclear Polarization Solid-State NMR in Heterogeneous Catalysis Research. ACS Catalysis, 2015, 5, 7055-7062.	11.2	160
4	Surface Termination of CsPbBr <sub>3</sub> Perovskite Quantum Dots Determined by Solid-State NMR Spectroscopy. Journal of the American Chemical Society, 2020, 142, 6117-6127.	13.7	135
5	Natural Abundance <sup>17</sup> O DNP Two-Dimensional and Surface-Enhanced NMR Spectroscopy. Journal of the American Chemical Society, 2015, 137, 8336-8339.	13.7	126
6	Potent inhibition of ice recrystallization by low molecular weight carbohydrate-based surfactants and hydrogelators. Chemical Science, 2012, 3, 1408.	7.4	102
7	Zero Thermal Expansion in ZrMgMo <sub>3</sub> O <sub>12</sub> : NMR Crystallography Reveals Origins of Thermoelastic Properties. Chemistry of Materials, 2015, 27, 2633-2646.	6.7	90
8	QUEST—QUadrupolar Exact SoftWare: A fast graphical program for the exact simulation of NMR and NQR spectra for quadrupolar nuclei. Solid State Nuclear Magnetic Resonance, 2012, 45-46, 36-44.	2.3	77
9	DNP-Enhanced Ultrawideband Solid-State NMR Spectroscopy: Studies of Platinum in Metal-Organic Frameworks. Journal of Physical Chemistry Letters, 2016, 7, 2322-2327.	4.6	77
10	Direct Investigation of Covalently Bound Chlorine in Organic Compounds by Solid-State <sup>35</sup> Cl NMR Spectroscopy and Exact Spectral Line-Shape Simulations. Angewandte Chemie - International Edition, 2012, 51, 4227-4230.	13.8	69
11	Probing Surface Hydrogen Bonding and Dynamics by Natural Abundance, Multidimensional, <sup>17</sup> O DNP-NMR Spectroscopy. Journal of Physical Chemistry C, 2016, 120, 11535-11544.	3.1	65
12	Natural Abundance <sup>17</sup> O DNP NMR Provides Precise O-H Distances and Insights into the Brønsted Acidity of Heterogeneous Catalysts. Angewandte Chemie - International Edition, 2017, 56, 9165-9169.	13.8	63
13	Characterizing Substrate-Surface Interactions on Alumina-Supported Metal Catalysts by Dynamic Nuclear Polarization-Enhanced Double-Resonance NMR Spectroscopy. Journal of the American Chemical Society, 2017, 139, 2702-2709.	13.7	59
14	Signal enhancement in solid-state NMR of quadrupolar nuclei. Solid State Nuclear Magnetic Resonance, 2013, 51-52, 1-15.	2.3	58
15	Atomic-Level Structure Characterization of Biomass Pre- and Post-Lignin Treatment by Dynamic Nuclear Polarization-Enhanced Solid-State NMR. Journal of Physical Chemistry A, 2017, 121, 623-630.	2.5	57
16	Chemoselective Hydrogenation with Supported Organoplatinum(IV) Catalyst on Zn(II)-Modified Silica. Journal of the American Chemical Society, 2018, 140, 3940-3951.	13.7	56
17	Multinuclear Magnetic Resonance Crystallographic Structure Refinement and Cross-Validation Using Experimental and Computed Electric Field Gradients: Application to Na <sub>2</sub> Al <sub>2</sub> B <sub>2</sub> O <sub>7</sub> . Journal of Physical Chemistry C, 2012, 116, 19472-19482.	3.1	52
18	Catalytic carbon-carbon bond cleavage and carbon-element bond formation give new life for polyolefins as biodegradable surfactants. Chem, 2021, 7, 1347-1362.	11.7	50

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19	Spying on the boron–boron triple bond using spin–spin coupling measured from <sup>11</sup> B solid-state NMR spectroscopy. <i>Chemical Science</i> , 2015, 6, 3378-3382.	7.4	47
20	Optimal sample formulations for DNP SENS: The importance of radical-surface interactions. <i>Current Opinion in Colloid and Interface Science</i> , 2018, 33, 9-18.	7.4	42
21	Boron–boron coupling constants are unique probes of electronic structure: a solid-state NMR and molecular orbital study. <i>Chemical Science</i> , 2014, 5, 2428-2437.	7.4	40
22	Sodium-23 Solid-State Nuclear Magnetic Resonance of Commercial Sodium Naproxen and its Solvates. <i>Journal of Pharmaceutical Sciences</i> , 2012, 101, 2930-2940.	3.3	39
23	Electrophilic Iridium(III) Pincer Complexes on Sulfated Zirconia for Hydrocarbon Activation and Functionalization. <i>Journal of the American Chemical Society</i> , 2019, 141, 6325-6337.	13.7	38
24	Identifying low-coverage surface species on supported noble metal nanoparticle catalysts by DNP-NMR. <i>Chemical Communications</i> , 2016, 52, 1859-1862.	4.1	36
25	Measuring dipolar and $J$ coupling between quadrupolar nuclei using double-rotation NMR. <i>Journal of Chemical Physics</i> , 2013, 138, 174202.	3.0	34
26	Effects of biradical deuteration on the performance of DNP: towards better performing polarizing agents. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 65-69.	2.8	34
27	Evidence for Redox Mechanisms in Organometallic Chemisorption and Reactivity on Sulfated Metal Oxides. <i>Journal of the American Chemical Society</i> , 2018, 140, 6308-6316.	13.7	34
28	PRESTO polarization transfer to quadrupolar nuclei: implications for dynamic nuclear polarization. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 22616-22622.	2.8	33
29	In Silico Design of DNP Polarizing Agents: Can Current Dinitroxides Be Improved?. <i>ChemPhysChem</i> , 2017, 18, 2279-2287.	2.1	32
30	Shedding light on the atomic-scale structure of amorphous silica–alumina and its Brønsted acid sites. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 19529-19537.	2.8	32
31	Symmetry-Amplified $J$ Splittings for Quadrupolar Spin Pairs: A Solid-State NMR Probe of Homoatomic Covalent Bonds. <i>Journal of the American Chemical Society</i> , 2013, 135, 12596-12599.	13.7	31
32	$t_1$ -Noise eliminated dipolar heteronuclear multiple-quantum coherence solid-state NMR spectroscopy. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 20815-20828.	2.8	31
33	Sterically Driven Olefin Metathesis: The Impact of Alkylidene Substitution on Catalyst Activity. <i>Organometallics</i> , 2016, 35, 691-698.	2.3	30
34	Site-Specific Sodiation Mechanisms of Selenium in Microporous Carbon Host. <i>Nano Letters</i> , 2020, 20, 918-928.	9.1	30
35	Surface Organometallic Chemistry of Supported Iridium(III) as a Probe for Organotransition Metal–Support Interactions in C–H Activation. <i>ACS Catalysis</i> , 2018, 8, 5363-5373.	11.2	29
36	Improved strategies for DNP-enhanced 2D 1H-X heteronuclear correlation spectroscopy of surfaces. <i>Solid State Nuclear Magnetic Resonance</i> , 2017, 87, 38-44.	2.3	27

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37	Direct <sup>17</sup> O dynamic nuclear polarization of single-site heterogeneous catalysts. <i>Chemical Communications</i> , 2018, 54, 3472-3475.	4.1	26
38	Two-step conversion of Kraft lignin to nylon precursors under mild conditions. <i>Green Chemistry</i> , 2020, 22, 4676-4682.	9.0	25
39	NMR crystallography of sodium diphosphates: combining dipolar, shielding, quadrupolar, diffraction, and computational information. <i>CrystEngComm</i> , 2013, 15, 8727.	2.6	24
40	Full-Scale Ab Initio Simulation of Magic-Angle-Spinning Dynamic Nuclear Polarization. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 5655-5660.	4.6	24
41	Large-scale <i>ab initio</i> simulations of MAS DNP enhancements using a Monte Carlo optimization strategy. <i>Journal of Chemical Physics</i> , 2018, 149, 154202.	3.0	22
42	Combining fast magic angle spinning dynamic nuclear polarization with indirect detection to further enhance the sensitivity of solid-state NMR spectroscopy. <i>Solid State Nuclear Magnetic Resonance</i> , 2020, 109, 101685.	2.3	22
43	Residual dipolar coupling between quadrupolar nuclei under magic-angle spinning and double-rotation conditions. <i>Journal of Magnetic Resonance</i> , 2011, 213, 82-89.	2.1	21
44	Direct Characterization of Metal-Metal Bonds between Nuclei with Strong Quadrupolar Interactions via NMR Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 4049-4054.	4.6	21
45	Theoretical study of homonuclear J coupling between quadrupolar spins: Single-crystal, DOR, and J-resolved NMR. <i>Journal of Magnetic Resonance</i> , 2014, 242, 23-32.	2.1	19
46	High-Field Magic Angle Spinning Dynamic Nuclear Polarization Using Radicals Created by <sup>13</sup> Irradiation. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4770-4776.	4.6	19
47	Condensed Phase Deactivation of Solid Brønsted Acids in the Dehydration of Fructose to Hydroxymethylfurfural. <i>ACS Catalysis</i> , 2019, 9, 11568-11578.	11.2	19
48	<sup>23</sup> Na double-rotation NMR of sodium nucleotides leads to the discovery of a new dCMP hendecahydrate. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 4677.	2.8	18
49	High sensitivity and resolution in <sup>43</sup> Ca solid-state NMR experiments. <i>Canadian Journal of Chemistry</i> , 2015, 93, 799-807.	1.1	18
50	Solid-state <sup>185/187</sup> Re NMR and GIPAW DFT study of perrhenates and Re <sub>2</sub> (CO) <sub>10</sub> : chemical shift anisotropy, NMR crystallography, and a metal-metal bond. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 10118-10134.	2.8	18
51	Observation of CH...N Interactions between Methyl and Carbonyl Groups in Proteins. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 7564-7567.	13.8	17
52	Synthesis of Supported Pd <sup>0</sup> Nanoparticles from a Single-Site Pd <sup>2+</sup> Surface Complex by Alkene Reduction. <i>Chemistry of Materials</i> , 2018, 30, 1032-1044.	6.7	17
53	Synthesis-enabled exploration of chiral and polar multivalent quaternary sulfides. <i>Chemical Science</i> , 2021, 12, 14718-14730.	7.4	16
54	Third time's the charm: intricate non-centrosymmetric polymorphism in Ln <sub>3</sub> SiP <sub>3</sub> (Ln = La and Ce) induced by distortions of phosphorus square layers. <i>Dalton Transactions</i> , 2021, 50, 6463-6476.	3.3	15

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55	Measurement of $^1J(199\text{Hg}, 31\text{P})$ in $[\text{HgPCy}_3(\text{OAc})_2]_2$ and relativistic ZORA DFT investigations of mercury-phosphorus coupling tensors. <i>Solid State Nuclear Magnetic Resonance</i> , 2009, 36, 182-191.	2.3	13
56	$^{23}\text{Na}$ magic-angle spinning and double-rotation NMR study of solid forms of sodium valproate. <i>Canadian Journal of Chemistry</i> , 2014, 92, 9-15.	1.1	13
57	Methyl-Driven Overhauser Dynamic Nuclear Polarization. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 4000-4006.	4.6	13
58	Dynamic Nuclear Polarization of Metal-Doped Oxide Glasses: A Test of the Generality of Paramagnetic Metal Polarizing Agents. <i>Journal of Physical Chemistry C</i> , 2020, 124, 23126-23133.	3.1	12
59	Direct determination of cellulosic glucan content in starch-containing samples. <i>Cellulose</i> , 2021, 28, 1989-2002.	4.9	12
60	Enhanced $1\text{H-X}$ D-HMQC performance through improved $1\text{H}$ homonuclear decoupling. <i>Solid State Nuclear Magnetic Resonance</i> , 2019, 98, 12-18.	2.3	11
61	Revealing the Configuration and Conformation of Surface Organometallic Catalysts with DNP-Enhanced NMR. <i>Journal of Physical Chemistry C</i> , 2021, 125, 13433-13442.	3.1	11
62	Determination of the chemical shift tensor anisotropy and asymmetry of strongly dipolar coupled protons under fast MAS. <i>Solid State Nuclear Magnetic Resonance</i> , 2021, 114, 101743.	2.3	11
63	Magnetic resonance imaging of DNP enhancements in a rotor spinning at the magic angle. <i>Journal of Magnetic Resonance</i> , 2016, 264, 125-130.	2.1	10
64	Quantitative structure parameters from the NMR spectroscopy of quadrupolar nuclei. <i>Pure and Applied Chemistry</i> , 2016, 88, 95-111.	1.9	10
65	Natural Abundance $^{17}\text{O}$ DNP...NMR Provides Precise $\text{O-H}$ Distances and Insights into the Brønsted Acidity of Heterogeneous Catalysts. <i>Angewandte Chemie</i> , 2017, 129, 9293-9297.	2.0	10
66	Hybrid quantum-classical simulations of magic angle spinning dynamic nuclear polarization in very large spin systems. <i>Journal of Chemical Physics</i> , 2022, 156, 124112.	3.0	10
67	Linear-scaling <i>ab initio</i> simulations of spin diffusion in rotating solids. <i>Journal of Chemical Physics</i> , 2019, 151, 034110.	3.0	9
68	Efficiency analysis of helium-cooled MAS DNP: case studies of surface-modified nanoparticles and homogeneous small-molecule solutions. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 4919-4926.	2.8	9
69	Observing the three-dimensional dynamics of supported metal complexes. <i>Inorganic Chemistry Frontiers</i> , 2021, 8, 1416-1431.	6.0	9
70	Activation of Low-Valent, Multiply $\sigma$ -Bonded Group VI Dimers toward Catalytic Olefin Metathesis via Surface Organometallic Chemistry. <i>Organometallics</i> , 2020, 39, 1035-1045.	2.3	8
71	Determining the Three-Dimensional Structures of Silica-Supported Metal Complexes from the Ground Up. <i>Inorganic Chemistry</i> , 2022, 61, 1067-1078.	4.0	8
72	A Heterogeneous Palladium Catalyst for the Polymerization of Olefins Prepared by Halide Abstraction Using Surface $\text{R}_3\text{Si}^+$ Species. <i>Angewandte Chemie</i> , 2022, 134, .	2.0	7

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73	Observation of CH <sub>2</sub> ...C=O Interactions between Methyl and Carbonyl Groups in Proteins. <i>Angewandte Chemie</i> , 2017, 129, 7672-7675.	2.0	5
74	Removal of sidebands in double-rotation NMR in real time. <i>Journal of Magnetic Resonance</i> , 2011, 211, 234-239.	2.1	3
75	Phase-sensitive <sup>13</sup> C-encoded recoupling of heteronuclear dipolar interactions and <sup>1</sup> H chemical shift anisotropy. <i>Solid State Nuclear Magnetic Resonance</i> , 2021, 111, 101712.	2.3	3
76	A ZORA-DFT and NLMO study of the one-bond fluorine-X indirect nuclear spin-spin coupling tensors for various VSEPR geometries. <i>Canadian Journal of Chemistry</i> , 2011, 89, 789-802.	1.1	2
77	Evolution of structure and transport properties of the Ba <sub>8</sub> Cu <sub>16</sub> P <sub>30</sub> clathrate-I framework with the introduction of Ga. <i>Applied Physics Letters</i> , 2022, 120, .	3.3	2
78	The anomalous solidification of concrete grindings from acid treatment. <i>Cement and Concrete Research</i> , 2019, 116, 65-69.	11.0	1
79	High Field Solid-State NMR of Challenging Nuclei in Inorganic Systems. , 2021, , .		1
80	Multifunctional Separator Allows Stable Cycling of Potassium Metal Anodes and of Potassium Metal Batteries ( <i>Adv. Mater.</i> 7/2022). <i>Advanced Materials</i> , 2022, 34, .	21.0	1
81	Innentitelbild: Natural Abundance <sup>17</sup> O DNP...NMR Provides Precise O-H Distances and Insights into the Brønsted Acidity of Heterogeneous Catalysts ( <i>Angew. Chem.</i> 31/2017). <i>Angewandte Chemie</i> , 2017, 129, 9032-9032.	2.0	0