Ilya Kuprov

List of Publications by Year
in descending order

95 papers	3,681 citations	126907 33 h-index	138484 58 g-index
99 all docs	99 docs citations	99 times ranked	3425 citing authors

#	Article	IF	Citations
1	Training SchrÃ¶dingerâ€™s cat: quantum optimal control. European Physical Journal D, 2015, 69, 1.	1.3	550
2	Spinach â€“ A software library for simulation of spin dynamics in large spin systems. Journal of Magnetic Resonance, 2011, 208, 179-194.	2.1	355
3	Second order gradient ascent pulse engineering. Journal of Magnetic Resonance, 2011, 212, 412-417.	2.1	210
4	Deep neural network processing of DEER data. Science Advances, 2018, 4, eaat5218.	10.3	134
5	Benchmark Test and Guidelines for DEER/PELDOR Experiments on Nitroxide-Labeled Biomolecules. Journal of the American Chemical Society, 2021, 143, 17875-17890.	13.7	124
6	How the Ligand Field in Lanthanide Coordination Complexes Determines Magnetic Susceptibility Anisotropy, Paramagnetic NMR Shift, and Relaxation Behavior. Accounts of Chemical Research, 2020, 53, 1520-1534.	15.6	109
7	Design Principles and Theory of Paramagnetic Fluorineâ€Labelled Lanthanide Complexes as Probes for ¹⁹F Magnetic Resonance: A Proofâ€ofâ€Concept Study. Chemistry - A European Journal, 2010, 16, 134-148.	3.3	98
8	Bidirectional Electron Transfer in Photosystem I:â€‰ Determination of Two Distances between P700+ and A1- in Spin-Correlated Radical Pairs. Biochemistry, 2005, 44, 2119-2128.	2.5	90
9	Aromatic 19F-13C TROSY: a background-free approach to probe biomolecular structure, function, and dynamics. Nature Methods, 2019, 16, 333-340.	19.0	82
10	1H line width dependence on MAS speed in solid state NMR â€“ Comparison of experiment and simulation. Journal of Magnetic Resonance, 2018, 291, 32-39.	2.1	80
11	19F NMR based pH probes: lanthanide(iii) complexes with pH-sensitive chemical shifts. Chemical Communications, 2008, , 2514.	4.1	79
12	Polynomially scaling spin dynamics simulation algorithm based on adaptive state-space restriction. Journal of Magnetic Resonance, 2007, 189, 241-250.	2.1	77
13	19F NMR Studies of the Native and Denatured States of Green Fluorescent Protein. Journal of the American Chemical Society, 2006, 128, 10729-10737.	13.7	61
14	Toroidal circular dichroism. Physical Review B, 2016, 94, .	3.2	57
15	Rationalization of Anomalous Pseudocontact Shifts and Their Solvent Dependence in a Series ofC₃-Symmetric Lanthanide Complexes. Journal of the American Chemical Society, 2017, 139, 14166-14172.	13.7	55
16	Polynomially scaling spin dynamics II: Further state-space compression using Krylov subspace techniques and zero track elimination. Journal of Magnetic Resonance, 2008, 195, 45-51.	2.1	52
17	Spatially encoded 2D and 3D diffusion-ordered NMR spectroscopy. Chemical Communications, 2017, 53, 701-704.	4.1	48
18	Uniform illumination of optically dense NMR samples. Journal of Magnetic Resonance, 2004, 171, 171-175.	2.1	46

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19	Modified Newton-Raphson GRAPE methods for optimal control of spin systems. Journal of Chemical Physics, 2016, 144, 204107.	3.0	46
20	Strategies for state space restriction in densely coupled spin systems with applications to spin chemistry. Journal of Chemical Physics, 2010, 132, 174101.	3.0	42
21	Heterometallic Zn₃Ln₃ Ensembles Containing (Î¼₆â€CO₃) Ligand and Triangular Disposition of Ln³⁺ ions: Analysis of Singleâ€Molecule Toroic (SMT) and Singleâ€Molecule Magnet (SMM) Behavior. Chemistry - A European Journal, 2017, 23, 16621-16636.	3.3	42
22	Beyond Bleaney's Theory: Experimental and Theoretical Analysis of Periodic Trends in Lanthanideâ€Induced Chemical Shift. Angewandte Chemie - International Edition, 2017, 56, 12215-12218.	13.8	42
23	Diagonalization-free implementation of spin relaxation theory for large spin systems. Journal of Magnetic Resonance, 2011, 209, 31-38.	2.1	41
24	Auxiliary matrix formalism for interaction representation transformations, optimal control, and spin relaxation theories. Journal of Chemical Physics, 2015, 143, 084113.	3.0	41
25	Lanthanide-induced relaxation anisotropy. Physical Chemistry Chemical Physics, 2018, 20, 17676-17686.	2.8	41
26	Conformational analysis of small organic molecules using NOE and RDC data: A discussion of strychnine and Î± -methylene- Î³ -butyrolactone. Journal of Magnetic Resonance, 2015, 261, 101-109.	2.1	40
27	Bloch-Redfield-Wangsness theory engine implementation using symbolic processing software. Journal of Magnetic Resonance, 2007, 184, 196-206.	2.1	39
28	Fokker-Planck formalism in magnetic resonance simulations. Journal of Magnetic Resonance, 2016, 270, 124-135.	2.1	39
29	Pseudocontact shifts from mobile spin labels. Physical Chemistry Chemical Physics, 2016, 18, 26412-26422.	2.8	39
30	On the accuracy of the state space restriction approximation for spin dynamics simulations. Journal of Chemical Physics, 2011, 135, 084106.	3.0	36
31	Constructive quantum interference in a bis-copper six-porphyrin nanoring. Nature Communications, 2017, 8, 14842.	12.8	36
32	A partial differential equation for pseudocontact shift. Physical Chemistry Chemical Physics, 2014, 16, 20184-20189.	2.8	35
33	PARASHIFT Probes: Solution NMR and X-ray Structural Studies of Macrocyclic Ytterbium and Yttrium Complexes. Inorganic Chemistry, 2017, 56, 4028-4038.	4.0	34
34	Optimal control of Raman pulse sequences for atom interferometry. Journal of Physics B: Atomic, Molecular and Optical Physics, 2020, 53, 085006.	1.5	33
35	Chemically amplified 19Fâ€“1H nuclear Overhauser effects. Journal of Magnetic Resonance, 2004, 168, 1-7.	2.1	32
36	¹⁴N overtone NMR under MAS: signal enhancement using symmetry-based sequences and novel simulation strategies. Physical Chemistry Chemical Physics, 2015, 17, 6577-6587.	2.8	32

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37	Optimal control of mirror pulses for cold-atom interferometry. Physical Review A, 2018, 98, .	2.5	32
38	Quantum mechanical NMR simulation algorithm for protein-size spin systems. Journal of Magnetic Resonance, 2014, 243, 107-113.	2.1	28
39	Minimising conformational bias in fluoroprolines through vicinal difluorination. Chemical Communications, 2018, 54, 5118-5121.	4.1	28
40	Model-free extraction of spin label position distributions from pseudocontact shift data. Chemical Science, 2017, 8, 2751-2757.	7.4	26
41	Exact NMR simulation of protein-size spin systems using tensor train formalism. Physical Review B, 2014, 90, .	3.2	24
42	Time domain simulation of Gd3+â€“Gd3+ distance measurements by EPR. Journal of Chemical Physics, 2017, 147, 044201.	3.0	23
43	Spin Relaxation Effects in Photochemically Induced Dynamic Nuclear Polarization Spectroscopy of Nuclei with Strongly Anisotropic Hyperfine Couplings. Journal of the American Chemical Society, 2007, 129, 9004-9013.	13.7	21
44	Neural network interpretation using descrambler groups. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	21
45	Quantitative analysis of 14N quadrupolar coupling using 1H detected 14N solid-state NMR. Physical Chemistry Chemical Physics, 2019, 21, 5941-5949.	2.8	20
46	Design and performance of a microsecond time-resolved photo-chemically induced dynamic nuclear polarization add-on for a high-field nuclear magnetic resonance spectrometer. Review of Scientific Instruments, 2005, 76, 084103.	1.3	19
47	Grid-free powder averages: On the applications of the Fokkerâ€“Planck equation to solid state NMR. Journal of Magnetic Resonance, 2013, 235, 121-129.	2.1	19
48	Using Paramagnetism to Slow Down Nuclear Relaxation in Protein NMR. Journal of Physical Chemistry Letters, 2016, 7, 4815-4818.	4.6	19
49	Understanding Jâ€Modulation during Spatial Encoding for Sensitivityâ€Optimized Ultrafast NMR Spectroscopy. ChemPhysChem, 2015, 16, 3093-3100.	2.1	18
50	Largeâ€scale <scp>NMR</scp> simulations in liquid state: A tutorial. Magnetic Resonance in Chemistry, 2018, 56, 415-437.	1.9	18
51	Neural networks in pulsed dipolar spectroscopy: A practical guide. Journal of Magnetic Resonance, 2022, 338, 107186.	2.1	18
52	Anomalous Nuclear Overhauser Effects in Carbonâ€Substituted Aziridines: Scalar Crossâ€Relaxation of the First Kind. Angewandte Chemie - International Edition, 2015, 54, 3697-3701.	13.8	17
53	Quantifying the exchange coupling in linear copper porphyrin oligomers. Physical Chemistry Chemical Physics, 2017, 19, 16057-16061.	2.8	17
54	Beyond Bleaney's Theory: Experimental and Theoretical Analysis of Periodic Trends in Lanthanideâ€Induced Chemical Shift. Angewandte Chemie, 2017, 129, 12383-12386.	2.0	17

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55	Observability of Paramagnetic NMR Signals at over 10â€‰000 ppm Chemical Shifts. Angewandte Chemie - International Edition, 2021, 60, 22856-22864.	13.8	17
56	Efficient simulation of ultrafast magnetic resonance experiments. Physical Chemistry Chemical Physics, 2017, 19, 17577-17586.	2.8	16
57	Synthesis and Conformational Properties of 3,4-Difluoro-<scp>l</scp>-prolines. Journal of Organic Chemistry, 2019, 84, 3100-3120.	3.2	16
58	Feedback control optimisation of ESR experiments. Journal of Magnetic Resonance, 2018, 297, 9-16.	2.1	14
59	Biselective pulses for large-area atom interferometry. Physical Review A, 2020, 101, .	2.5	14
60	Novel pulse sequences for time-resolved photo-CIDNP. Molecular Physics, 2006, 104, 1675-1686.	1.7	13
61	¹⁴N overtone transition in double rotation solid-state NMR. Physical Chemistry Chemical Physics, 2015, 17, 23748-23753.	2.8	13
62	Periodic trends and hidden dynamics of magnetic properties in three series of triazacyclononane lanthanide complexes. Dalton Transactions, 2019, 48, 8400-8409.	3.3	13
63	Destination state screening of active spaces in spin dynamics simulations. Journal of Magnetic Resonance, 2011, 210, 228-232.	2.1	12
64	Transmembrane Exchange of Fluorosugars: Characterization of Red Cell GLUT1 Kinetics UsingÂ19F NMR. Biophysical Journal, 2018, 115, 1906-1919.	0.5	12
65	A standard format and a graphical user interface for spin system specification. Journal of Magnetic Resonance, 2014, 240, 124-131.	2.1	11
66	Measurement of 14N quadrupole couplings in biomolecular solids using indirect-detection 14N solid-state NMR with DNP. Chemical Communications, 2017, 53, 12116-12119.	4.1	11
67	Photoionization of TMPD in DMSO solution: mechanism and magnetic field effects. Molecular Physics, 2006, 104, 1789-1794.	1.7	10
68	Parallel density matrix propagation in spin dynamics simulations. Journal of Chemical Physics, 2012, 136, 044108.	3.0	10
69	Spin system trajectory analysis under optimal control pulses. Journal of Magnetic Resonance, 2013, 233, 107-112.	2.1	10
70	Benchmarking NMR experiments: A relational database of protein pulse sequences. Journal of Magnetic Resonance, 2010, 203, 129-137.	2.1	9
71	Separating the coherence transfer from chemical shift evolution in highâ€resolution pure shift <scp>COSY NMR</scp>. Magnetic Resonance in Chemistry, 2018, 56, 969-975.	1.9	8
72	Quantum mechanical MRI simulations: Solving the matrix dimension problem. Science Advances, 2019, 5, eaaw8962.	10.3	8

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73	High-field solution state DNP using cross-correlations. Journal of Magnetic Resonance, 2021, 326, 106940.	2.1	7
74	Second order phase dispersion by optimized rotation pulses. Physical Review Research, 2020, 2, .	3.6	6
75	J-Driven dynamic nuclear polarization for sensitizing high field solution state NMR. Physical Chemistry Chemical Physics, 2022, 24, 2118-2125.	2.8	6
76	Theoretical analysis of scalar relaxation in 13C-DNP in liquids. Journal of Magnetic Resonance Open, 2022, 10-11, 100040.	1.1	6
77	Indirect detection of 10B (Iâ€¯=â€¯3) overtone NMR at very fast magic angle spinning. Journal of Magnetic Resonance, 2018, 291, 27-31.	2.1	5
78	Concurrent J-Evolving Refocusing Pulses. Journal of Magnetic Resonance, 2022, 336, 107152.	2.1	5
79	SORDOR pulses: expansion of the BÃ¶hlenâ€“Bodenhausen scheme for low-power broadband magnetic resonance. Magnetic Resonance, 2022, 3, 53-63.	1.9	5
80	Molecular structure refinement by direct fitting of atomic coordinates to experimental ESR spectra. Journal of Magnetic Resonance, 2012, 216, 62-68.	2.1	4
81	Scalar Cross-Relaxation Detected in the NOESY Spectra of Oxazolidines and Thiazolidines. Journal of Organic Chemistry, 2016, 81, 4142-4148.	3.2	4
82	Defeating the Matrix. Journal of Magnetic Resonance, 2019, 306, 75-79.	2.1	4
83	Using molecular dynamics trajectories to predict nuclear spin relaxation behaviour in large spin systems. Journal of Magnetic Resonance, 2021, 323, 106891.	2.1	4
84	Measuring Spin Relaxation Rates Using Satellite Exchange NMR Spectroscopy. Angewandte Chemie - International Edition, 2018, 57, 7498-7502.	13.8	3
85	Combining Molecular and Spin Dynamics Simulations with Solid-State NMR: A Case Study of Amphiphilic Lysineâ€“Leucine Repeat Peptide Aggregates. Journal of Physical Chemistry B, 2019, 123, 10915-10929.	2.6	3
86	14N overtone NMR under MAS: Signal enhancement using cross-polarization methods. Journal of Magnetic Resonance, 2019, 298, 1-5.	2.1	3
87	Heteronuclear transfers from labile protons in biomolecular NMR: Cross polarization, revisited. Journal of Magnetic Resonance, 2021, 333, 107083.	2.1	3
88	Optimal control gradient precision trade-offs: application to fast generation of DeepControl libraries for MRI. Journal of Magnetic Resonance, 2021, 333, 107094.	2.1	3
89	Fluorine NMR study of proline-rich sequences using fluoroprolines. Magnetic Resonance, 2021, 2, 795-813.	1.9	3
90	Coherence transfer delay optimisation in PSYCOSY experiments. Magnetic Resonance in Chemistry, 2020, 58, 51-55.	1.9	1

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91	Strategies for 1 Hâ€Detected Dynamic Nuclear Polarization Magicâ€Angle Spinning NMR Spectroscopy. Chemistry - A European Journal, 2020, 26, 15852-15854.	3.3	1
92	Observability of paramagnetic NMR signals at over 10â€‰000 ppm chemical shifts. Angewandte Chemie, 2021, 133, 23038.	2.0	1
93	Spin Relaxation in Ru-Chromophore-Linked Azine/Diquat Radical Pairs. , 0, , 205-220.		0
94	Measuring Spin Relaxation Rates Using Satellite Exchange NMR Spectroscopy. Angewandte Chemie, 2018, 130, 7620-7624.	2.0	0
95	Can optimised pulses improve the sensitivity of atom interferometers?. , 2021, , .		0