

Aleksandr A Shubin

List of Publications by Year in descending order

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95
papers

1,925
citations

236833

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97
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#	ARTICLE	IF	CITATIONS
1	Entropy driven preference for alkene adsorption at the pore mouth as the origin of pore-mouth catalysis for alkane hydroisomerization in 1D zeolites. <i>Catalysis Science and Technology</i> , 2021, 11, 563-574.	2.1	5
2	Ln(III) complexes with a chiral 1 <i>H</i> -pyrazolo[3,4- <i>b</i>]pyridine derivative fused with a (â [~])- α -pinene moiety: synthesis, crystal structure, and photophysical studies in solution and in the solid state. <i>New Journal of Chemistry</i> , 2021, 45, 2276-2284.	1.4	5
3	Identification of beryllium fluoride complexes in mechanically distorted gels using quadrupolar split ⁹ Be NMR spectra resolved with solution-state selective cross-polarization. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16932-16941.	1.3	1
4	The impact of framework flexibility and defects on the water adsorption in CAU-10-H. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 21329-21337.	1.3	17
5	The Fe IV=O \rightarrow oxyl unit as a key intermediate in water oxidation on the Fe III hydroxide: DFT predictions. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26610.	1.0	0
6	Crystal structure of copper perchlorophthalocyanine analysed by 3D electron diffraction. <i>Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials</i> , 2021, 77, 662-675.	0.5	9
7	Investigation of vanadia α -alumina catalysts with solid-state NMR spectroscopy and DFT. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 19352-19363.	1.3	1
8	A novel adsorption-based method for revealing the Si distribution in SAPO molecular sieves: The case of SAPO-11. <i>Microporous and Mesoporous Materials</i> , 2021, 328, 111503.	2.2	5
9	Condensation of ammonium niobium oxalate studied by NMR crystallography and X-ray powder diffraction. <i>Catalysis Today</i> , 2020, 354, 26-35.	2.2	4
10	Oxygen transport in Pr nickelates: Elucidation of atomic-scale features. <i>Solid State Ionics</i> , 2020, 344, 115155.	1.3	6
11	Integral Intensity of the EPR Signal of NO Molecules Adsorbed on Lewis Acid Sites of Oxide Systems as a Function of Surface Coverage. <i>Applied Magnetic Resonance</i> , 2020, 51, 993-1003.	0.6	0
12	Photochemistry of dithiophosphinate Ni(S ₂ P(i-Bu) ₂) ₂ complex in CCl ₄ . Transient species and TD-DFT calculations. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2019, 381, 111857.	2.0	3
13	Photophysical processes for phenanthroline-menthol ligand and its Eu(III) and Tb(III) complexes in solution. <i>Journal of Luminescence</i> , 2019, 214, 116548.	1.5	0
14	Oxidation of Water to Molecular Oxygen by One-Electron Oxidants on Transition Metal Hydroxides. <i>Kinetics and Catalysis</i> , 2018, 59, 23-47.	0.3	6
15	Hydrogen abstraction from methane on cristobalite supported W and Mn oxo complexes: A DFT study. <i>Molecular Catalysis</i> , 2018, 445, 307-315.	1.0	15
16	Pyrolysis of the Cellulose Fraction of Biomass in the Presence of Solid Acid Catalysts: An Operando Spectroscopy and Theoretical Investigation. <i>ChemSusChem</i> , 2018, 11, 4044-4059.	3.6	7
17	Influence of Polarity and Ionic Strength on Intramolecular Spin Exchange in a Short Nitroxide Biradical, Containing Sulphur Atom in the Bridge. <i>Applied Magnetic Resonance</i> , 2018, 49, 1059-1073.	0.6	3
18	Solid-State NMR of Oxide-Based Materials. , 2018, , 1125-1160.		2

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19	Hidden radical reactivity of the [FeO] ₂ ⁺ group in the H-abstraction from methane: DFT and CASPT2 supported mechanism by the example of model iron (hydro)oxide species. <i>Chemical Physics Letters</i> , 2017, 679, 193-199.	1.2	10
20	Surface Hydroxyl OH Defects of γ -Al ₂ O ₃ and δ -Al ₂ O ₃ by Solid State NMR, XRD, and DFT Calculations. <i>Zeitschrift Fur Physikalische Chemie</i> , 2017, 231, 809-825.	1.4	13
21	Solid-State NMR of Oxide-Based Materials. , 2016, , 1-37.		0
22	DFT predictions for hydrogen atom transfer at the [FeO] ₂ ⁺ group: A distinct activity of the oxyl state FeIII-O [•] . <i>AIP Conference Proceedings</i> , 2016, , .	0.3	1
23	Photochemistry of Dithiocarbamate Cu(S ₂ CNEt ₂) ₂ Complex in CHCl ₃ . Transient Species and TD-DFT Calculations. <i>Journal of Physical Chemistry A</i> , 2016, 120, 7873-7880.	1.1	7
24	Random Distribution of EFG Parameters in ²⁷ Al MAS NMR Spectra of AlO _x /SiO ₂ Catalysts and Related Systems. <i>Applied Magnetic Resonance</i> , 2016, 47, 1193-1205.	0.6	2
25	First principles calculation of the stacking fault in (111) low-temperature metastable alumina. <i>Journal of Structural Chemistry</i> , 2016, 57, 294-300.	0.3	3
26	Electron Paramagnetic Resonance Study of the Interaction of Surface Titanium Species with AlR ₃ Cocatalyst in Supported Ziegler-Natta Catalysts with a Low Titanium Content. <i>Journal of Physical Chemistry C</i> , 2016, 120, 1121-1129.	1.5	16
27	Effect of Impregnation on the Structure of Niobium Oxide/Alumina Catalysts Studied by Multinuclear Solid-State NMR, FTIR, and Quantum Chemical Calculations. <i>Journal of Physical Chemistry C</i> , 2015, 119, 10400-10411.	1.5	10
28	Distinct activity of the oxyl FeIII O group in the methane dissociation by activated iron hydroxide: DFT predictions. <i>Chemical Physics Letters</i> , 2015, 640, 94-100.	1.2	12
29	The routes of association of (hydro)oxo centers on iron hydroxide at the water oxidation process: DFT predictions. <i>Chemical Physics Letters</i> , 2015, 619, 126-132.	1.2	10
30	Raman identification of lonsdaleite in Popigai impactites. <i>Journal of Raman Spectroscopy</i> , 2014, 45, 305-313.	1.2	36
31	The structure of zirconium-silicate fibreglasses and Pt-containing fiberglass catalysts as revealed by solid-state NMR spectroscopy. <i>Journal of Structural Chemistry</i> , 2013, 54, 152-167.	0.3	5
32	Orbital ordering of Cu ²⁺ ions in concentrated aqueous ammonia solutions of copper chloride, sulfate, and acetate as probed by ESR. <i>Doklady Physical Chemistry</i> , 2013, 450, 103-106.	0.2	2
33	Theoretical and experimental insights into applicability of solid-state ⁹³ Nb NMR in catalysis. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 5115.	1.3	48
34	The state of Cu ²⁺ ions in concentrated aqueous ammonia solutions of copper nitrate. <i>Russian Journal of Inorganic Chemistry</i> , 2012, 57, 1285-1290.	0.3	10
35	Specific features of association of Cu ²⁺ ions in concentrated aqueous ammonia solutions of copper nitrate as probed by ESR. <i>Doklady Physical Chemistry</i> , 2011, 440, 194-197.	0.2	6
36	Exploring by Pulsed EPR the Electronic Structure of Ubisemiquinone Bound at the QH Site of Cytochrome bo ₃ from Escherichia coli with in Vivo ¹³ C-Labeled Methyl and Methoxy Substituents. <i>Journal of Biological Chemistry</i> , 2011, 286, 10105-10114.	1.6	20

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37	Self-Aggregation and Orientation of the Ion Channel-Forming Zervamicin IIA in the Membranes of ePC Vesicles Studied by cw EPR and ESEEM Spectroscopy. <i>Applied Magnetic Resonance</i> , 2010, 38, 75-84.	0.6	13
38	An EPR Study of the V(IV) Species Formed Upon Activation of a Vanadyl Phenoxyimine Polymerization Catalyst with AlR_3 and AlR_2Cl ($\text{R} = \text{Me}, \text{Et}$). <i>Macromolecular Chemistry and Physics</i> , 2009, 210, 542-548.	1.1	28
39	On the nature of radicals formed in methanol catalytic oxidation. <i>Kinetics and Catalysis</i> , 2009, 50, 583-586.	0.3	1
40	Solid-state ^{51}V NMR and its potentiality in investigation of vanadia systems with paramagnetic centres. <i>Catalysis Today</i> , 2009, 142, 220-226.	2.2	7
41	EPR Monitoring of Vanadium(IV) Species Formed upon Activation of Vanadium(V) Polyphenolate Precatalysts with AlR_2Cl and $\text{AlR}_2\text{Cl}/\text{Ethyltrichloroacetate}$ ($\text{R} = \text{Me}, \text{Et}$). <i>Organometallics</i> , 2009, 28, 6714-6720.	1.1	43
42	Proton Environment of Reduced Rieske Iron-Sulfur Cluster Probed by Two-Dimensional ESEEM Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2009, 113, 653-667.	1.1	19
43	Practical aspects of ^{51}V and ^{93}Nb solid-state NMR spectroscopy and applications to oxide materials. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 2008, 53, 128-191.	3.9	85
44	ESEEM Measurements of Local Water Concentration in D_2O -Containing Spin-Labeled Systems. <i>Applied Magnetic Resonance</i> , 2008, 35, 73-94.	0.6	35
45	Adsorption properties of oxidized gallium-modified zeolite ZSM-5 from diffuse-reflectance IR-spectroscopic and quantum-chemical data: II. Interaction with carbon monoxide and water. <i>Kinetics and Catalysis</i> , 2008, 49, 149-155.	0.3	3
46	Cluster Model DFT Study of CO Adsorption to Gallium Ions in Ga/HZSM-5. <i>Journal of Physical Chemistry C</i> , 2008, 112, 3321-3326.	1.5	17
47	Variations of g-tensor principal values in reduced $[\text{Fe}^{\text{II}}\text{S}_2]$ cluster of iron-sulfur proteins. <i>Applied Magnetic Resonance</i> , 2006, 30, 399-416.	0.6	6
48	Spectroscopic identification of adsorption properties of Zn^{2+} ions at cationic positions of high-silica zeolites with distant placing of aluminium ions. <i>Theoretical Chemistry Accounts</i> , 2005, 114, 90-96.	0.5	39
49	Water Concentration Profiles in Membranes Measured by ESEEM of Spin-Labeled Lipids. <i>Journal of Physical Chemistry B</i> , 2005, 109, 12003-12013.	1.2	116
50	A comparative, two-dimensional ^{14}N ESEEM characterization of reduced $[\text{Fe}^{\text{II}}\text{S}_2]$ clusters in hyperthermophilic archaeal high- and low-potential Rieske-type proteins. <i>Journal of Biological Inorganic Chemistry</i> , 2004, 9, 753-767.	1.1	25
51	Possible molecular structure of promoted Lewis acidity sites in ZnZSM-5. <i>International Journal of Quantum Chemistry</i> , 2004, 100, 489-494.	1.0	32
52	DFT Cluster Modeling of Molecular and Dissociative Hydrogen Adsorption on Zn^{2+} Ions with Distant Placing of Aluminum in the Framework of High-Silica Zeolites. <i>Catalysis Letters</i> , 2003, 90, 137-142.	1.4	45
53	Solid-state NMR for characterization of vanadium-containing systems. <i>Catalysis Today</i> , 2003, 78, 91-104.	2.2	41
54	Dynamics of n-Hexane Inside Silicalite, As Studied by ^2H NMR. <i>Journal of Physical Chemistry B</i> , 2003, 107, 7095-7101.	1.2	21

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55	Dynamics of Isobutane inside Zeolite ZSM-5. A Study with Deuterium Solid-State NMR. Journal of Physical Chemistry B, 2002, 106, 10114-10120.	1.2	25
56	Determination of Hyperfine Tensor Components from Nuclear Frequencies at Canonical Orientations of the g-Tensor. Journal of Magnetic Resonance, 2002, 155, 100-105.	1.2	1
57	EPR-spectroscopic detection and characterization of a CuII complex with a peroxycarboximidic acid. Mendeleev Communications, 2001, 11, 206-207.	0.6	1
58	Comparative Quantum Chemical Study of Stabilization Energies of Zn ²⁺ Ions in Different Zeolite Structures. Journal of Physical Chemistry B, 2001, 105, 4928-4935.	1.2	51
59	Antimony Oxide-Modified Vanadia-Based Catalysts Physical Characterization and Catalytic Properties. Journal of Physical Chemistry B, 2001, 105, 10772-10783.	1.2	49
60	Reactivity Theory of Zinc Cation Species in Zeolites. , 2001, , 187-204.		2
61	Observation of two paramagnetic species in electron transfer reactions within cesium modified X and Y zeolites. Chemical Physics Letters, 2000, 316, 404-410.	1.2	15
62	51V and 31P NMR studies of VO _x /TiO ₂ catalysts modified by phosphorous. Journal of Molecular Catalysis A, 2000, 162, 381-390.	4.8	30
63	Characterization by solid state 51V NMR spectroscopy. Catalysis Today, 2000, 56, 379-387.	2.2	26
64	DFT study of oxygen-bridged Zn ²⁺ ion pairs in Zn/ZSM-5 zeolites. Catalysis Letters, 2000, 70, 175-181.	1.4	83
65	Molecular Dynamics of iso-Butyl Alcohol Inside Zeolite H-ZSM-5 as Studied by Deuterium Solid-State NMR Spectroscopy. Journal of Physical Chemistry B, 2000, 104, 7677-7685.	1.2	20
66	High-temperature multinuclear magnetic resonance studies of vanadia catalysts for SO ₂ oxidation. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 1999, 158, 255-271.	2.3	9
67	The metallocene/methylaluminoxane catalysts formation: EPR spin probe study of Lewis acidic sites of methylaluminoxane. Journal of Molecular Catalysis A, 1999, 139, 131-137.	4.8	63
68	Characterisation of strongly bonded V(V) species in VO _x /TiO ₂ catalyst by static and MAS solid-state NMR spectroscopy. Chemical Physics Letters, 1999, 302, 341-346.	1.2	41
69	Effect of Milling of V ₂ O ₅ on the Local Environment of Vanadium as Studied by Solid-State 51V NMR and Complementary Methods. Journal of Physical Chemistry B, 1999, 103, 3138-3144.	1.2	36
70	Characterization of V ₂ O ₅ /TiO ₂ Catalysts Prepared by Milling by ESR and Solid State 1H and 51V NMR. Journal of Physical Chemistry B, 1999, 103, 7599-7606.	1.2	51
71	Molecular Dynamics of n-Octane Inside Zeolite ZSM-5 As Studied by Deuterium Solid-State NMR and Quasi-Elastic Neutron Scattering. Journal of Physical Chemistry B, 1998, 102, 10860-10870.	1.2	32
72	High-Temperature NMR Studies of the Glass-Crystal Transition in the Cs ₂ S ₂ O ₇ /V ₂ O ₅ System. Journal of Physical Chemistry B, 1997, 101, 9188-9194.	1.2	14

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73	EPR and ¹ H NMR spectroscopic characterization of the ferric species formed in the iron picolinate/(pyridine/acetic acid)/HOOH catalytic system for the direct ketonization of methylenic carbons. <i>Journal of Molecular Catalysis A</i> , 1996, 112, 253-258.	4.8	13
74	Multinuclear NMR studies of V ₂ O ₅ -Cs ₂ S ₂ O ₇ melts. <i>Journal of Molecular Catalysis A</i> , 1995, 99, 123-130.	4.8	19
75	ESR study of ordered Ti(III) clusters in frozen solutions. <i>Reaction Kinetics and Catalysis Letters</i> , 1994, 52, 261-267.	0.6	1
76	A computational study of the adsorption of the isomers of butanol on silicalite and H-ZSM-5. <i>Proceedings of the Royal Society A</i> , 1994, 446, 411-427.	1.0	22
77	Radical Intermediates in the Photoinduced Formation of Benzene Cation-Radicals over H-ZSM-5 Zeolites. <i>The Journal of Physical Chemistry</i> , 1994, 98, 7551-7554.	2.9	36
78	ESR spectra of oxygen radical-ions in kaolinite. <i>Journal of Structural Chemistry</i> , 1992, 33, 151-153.	0.3	1
79	⁵¹ V Solid state NMR studies of vanadia based catalysts. <i>Progress in Nuclear Magnetic Resonance Spectroscopy</i> , 1992, 24, 457-525.	3.9	180
80	Relation between catalyst structure and selectivity of the oxidative coupling of 2,6-dimethylphenol in the presence of copper complexes: studies using EPR and NMR. <i>Journal of Molecular Catalysis</i> , 1990, 57, 325-351.	1.2	25
81	Composition of the active component of supported vanadium-magnesium catalysts according to ⁵¹ V NMR data. <i>Journal of Molecular Catalysis</i> , 1989, 50, 55-65.	1.2	44
82	Calculation of anisotropically broadened EPR spectra. Shape of the EPR spectrum of a nitroxide radical in the two-millimeter range. <i>Journal of Structural Chemistry</i> , 1989, 30, 414-417.	0.3	10
83	Spatial organization of random coils of linear poly(ethylenimine) containing copper(II) ions in solution. <i>Journal of Structural Chemistry</i> , 1989, 30, 260-267.	0.3	0
84	²³ Na NMR study of the mechanism for the dehydration of zeolite NaA. <i>Bulletin of the Academy of Sciences of the USSR Division of Chemical Science</i> , 1988, 37, 1020-1022.	0.0	2
85	Formation, structure, and reactivity of palladium superoxo complexes. <i>Inorganic Chemistry</i> , 1987, 26, 3871-3878.	1.9	13
86	High-resolution solid-state magic angle spinning nuclear magnetic resonance investigations of surface hydroxy groups on modified silica gel. <i>Journal of the Chemical Society Faraday Transactions I</i> , 1986, 82, 1879.	1.0	22
87	Factors affecting the stability and selectivity of zeolites in the conversion of methanol to hydrocarbons. Communication 2. Effect of dealuminization. <i>Bulletin of the Academy of Sciences of the USSR Division of Chemical Science</i> , 1986, 35, 909-913.	0.0	1
88	O ₂ ^{•-} anion radical in the coordination sphere of palladium in solution. <i>Reaction Kinetics and Catalysis Letters</i> , 1986, 31, 209-214.	0.6	5
89	Numerical analysis of the influence of nuclear quadrupole interaction on modulation effects in electron spin echo from deuterium nuclei in disordered systems. <i>Journal of Magnetic Resonance</i> , 1985, 64, 185-193.	0.5	6
90	Study of nature of the factors determining activity, stability and selectivity of zeolite catalyst. <i>Zeolites</i> , 1984, 4, 114-119.	0.9	21

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91	The influence of nuclear quadrupole interactions upon electron spin-echo modulation induced by weak hyperfine interactions. <i>Journal of Magnetic Resonance</i> , 1983, 52, 1-12.	0.5	17
92	Electron spin-echo modulation effects in disordered systems: Structure of traps for H and D atoms in frozen water solutions based on ^1H and ^2D nuclear modulation data. <i>Journal of Chemical Physics</i> , 1983, 79, 5785-5795.	1.2	12
93	A study of polyhedral octa (organosilasesquioxanes) by high-resolution NMR at the ^{13}C and ^{29}Si nuclei in the solid state. <i>Journal of Structural Chemistry</i> , 1982, 23, 345-348.	0.3	4
94	Modulation effects in the electron spin echo resulting from hyperfine interaction with a nucleus of an arbitrary spin. <i>Journal of Magnetic Resonance</i> , 1981, 42, 474-487.	0.5	44
95	Change in sign of exchange integral in conformational transition in molecule of stable nitroxyl diradical. <i>Bulletin of the Academy of Sciences of the USSR Division of Chemical Science</i> , 1981, 30, 1660-1663.	0.0	2