

# JÃ¼rgen Schnack

## List of Publications by Year in descending order

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136  
papers

3,897  
citations

136885

32  
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138  
all docs

138  
docs citations

138  
times ranked

3009  
citing authors

#	ARTICLE	IF	CITATIONS
1	Polyoxometalates: Fascinating structures, unique magnetic properties. Coordination Chemistry Reviews, 2009, 253, 2315-2327.	9.5	508
2	Molecular dynamics for fermions. Reviews of Modern Physics, 2000, 72, 655-688.	16.4	189
3	Classical and Quantum Magnetism in Giant Keplerate Magnetic Molecules. ChemPhysChem, 2001, 2, 517-521.	1.0	180
4	The Importance of Being Exchanged: [Gd <sup>III</sup> ] <sub>4</sub> M <sup>II</sup> <sub>8</sub> (OH) <sub>8</sub> (L) <sub>8</sub> (O) <sub>2</sub> (CR) <sub>8</sub> Clusters for Magnetic Refrigeration. Angewandte Chemie - International Edition, 2012, 51, 4633-4636.	1.7	78
5	Effects of frustration on magnetic molecules: a survey from Olivier Kahn until today. Dalton Transactions, 2010, 39, 4677.	1.6	156
6	Quantum signatures of a molecular nanomagnet in direct magnetocaloric measurements. Nature Communications, 2014, 5, 5321.	5.8	115
7	Enhanced magnetocaloric effect in frustrated magnetic molecules with icosahedral symmetry. Physical Review B, 2007, 76, .	1.1	88
8	Magnetic characterization of the frustrated three-leg ladder compound [(CuCl <sub>2</sub> tachH) <sub>3</sub> Cl]Cl <sub>2</sub> . Physical Review B, 2004, 70, .	1.1	86
9	High spin cycles: topping the spin record for a single molecule verging on quantum criticality. Npj Quantum Materials, 2018, 3, .	1.8	86
10	Competing Spin Phases in Geometrically Frustrated Magnetic Molecules. Physical Review Letters, 2005, 94, 017205.	2.9	85
11	Exchange Interactions and Zero-Field Splittings in <i>C</i> <sub>3</sub> -Symmetric Mn <sup>III</sup> <sub>6</sub> Fe <sup>III</sup> : Using Molecular Recognition for the Construction of a Series of High Spin Complexes Based on the Triplesalen Ligand. Inorganic Chemistry, 2009, 48, 607-620.	1.9	75
12	Molybdate templated assembly of Ln <sub>12</sub> Mo <sub>4</sub> -type clusters (Ln = Sm, Eu, Gd) containing a truncated tetrahedron core. Chemical Communications, 2013, 49, 36-38.	2.2	72
13	Magnetism of the $\text{N}^{\text{II}}\text{Mn}^{\text{II}}\text{O}_{12}$ lattice antiferromagnet. Physical Review B, 2018, 98, .	1.4	42
14	Properties of highly frustrated magnetic molecules studied by the finite-temperature Lanczos method. European Physical Journal B, 2010, 78, 535-541.	0.6	70
15	Metamagnetic Phase Transition of the Antiferromagnetic Heisenberg Icosahedron. Physical Review Letters, 2005, 94, 207203.	2.9	59
16	Calculating the energy spectra of magnetic molecules: application of real- and spin-space symmetries. International Reviews in Physical Chemistry, 2010, 29, 403-452.	0.9	56
17	Iron Lanthanide Phosphonate Clusters: {Fe <sub>6</sub> Ln <sub>6</sub> P <sub>6</sub> } Wells-like Dawson-like Structures with <i>D</i> <sub>3d</sub> Symmetry. Inorganic Chemistry, 2014, 53, 3032-3038.	1.9	52
18	Numerically exact and approximate determination of energy eigenvalues for antiferromagnetic molecules using irreducible tensor operators and general point-group symmetries. Physical Review B, 2009, 79, .	1.1	49

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19	Quantum numbers for relative ground states of antiferromagnetic Heisenberg spin rings. Physical Review B, 2003, 68, .	1.1	48
20	Heat Capacity Reveals the Physics of a Frustrated Spin Tube. Physical Review Letters, 2010, 105, 037206.	2.9	45
21	Evaluation of the low-lying energy spectrum of magnetic Keplerate molecules using the density-matrix renormalization group technique. Physical Review B, 2003, 67, .	1.1	42
22	Observation of the influence of dipolar and spin frustration effects on the magnetocaloric properties of a trigonal prismatic $\{Gd_{7}\}$ molecular nanomagnet. Chemical Science, 2016, 7, 4891-4895.	3.7	42
23	Octametallic 4f-phosphonate horseshoes. Dalton Transactions, 2013, 42, 14045.	1.6	39
24	Centred nine-metal rings of lanthanides. Chemical Communications, 2014, 50, 1438-1440.	2.2	39
25	Discrete antiferromagnetic spin-wave excitations in the giant ferric wheel Fe <sub>18</sub> . Physical Review B, 2012, 86, .	1.1	38
26	Strong and Anisotropic Superexchange in the Single-Molecule Magnet (SMM) $[Mn^{III}_6Os^{III}_3]^{3+}$ : Promoting SMM Behavior through 3d-5d Transition Metal Substitution. Inorganic Chemistry, 2014, 53, 257-268.	1.9	38
27	Accuracy of the finite-temperature Lanczos method compared to simple typicality-based estimates. Physical Review Research, 2020, 2, .	1.3	38
28	Hysteresis in the ground and excited spin state up to 10 T of a $[Mn^{III}_6Mn^{III}]_3^{3+}$ triplesalen single-molecule magnet. Chemical Science, 2012, 3, 2868.	3.7	37
29	Observation of field-dependent magnetic parameters in the magnetic molecule $\{Ni_4Mo_{12}\}$ . Physical Review B, 2006, 73, .	1.1	35
30	A Star-Shaped Heteronuclear $Cr^{III}_3Mn^{II}_3$ Species and Its Precise Electronic and Magnetic Structure: Spin Frustration Studied by X-Ray Spectroscopic, Magnetic, and Theoretical Methods. Inorganic Chemistry, 2010, 49, 2093-2102.	1.9	35
31	Structural influences on the exchange coupling and zero-field splitting in the single-molecule magnet $[Mn^{III}_6Mn^{III}]_3^{3+}$ . Dalton Transactions, 2012, 41, 12942.	1.6	34
32	Environmental Influence on the Single-Molecule Magnet Behavior of $[Mn^{III}_6Cr^{III}_3]^{3+}$ : Molecular Symmetry versus Solid-State Effects. Inorganic Chemistry, 2012, 51, 10929-10954.	1.9	33
33	Quantum tunneling of the magnetization in $[Mn^{III}_6M]_3^{3+}$ (M=Cr <sup>III</sup> , Mn <sup>III</sup> ) SMMs: Impact of molecular and crystal symmetry. Coordination Chemistry Reviews, 2015, 289-290, 261-278.	9.5	33
34	Large magnetic molecules and what we learn from them. Contemporary Physics, 2019, 60, 127-144.	0.8	32
35	Inorganic Approach to Stabilizing Nanoscale Toroidicity in a Tetraicosanuclear Fe <sub>18</sub> Dy <sub>6</sub> Single Molecule Magnet. Journal of the American Chemical Society, 2020, 142, 14838-14842.	6.6	32
36	Synthesis and Characterization of the Heptanuclear $[Mn^{III}_6Co^{III}]_3^{3+}$ Triplesalen Complex: Evidence for Exchange Pathways Involving Low-spin Co <sup>III</sup> . Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2010, 65, 295-303.	0.3	31

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37	A MnIII triplesalen-based 1D pearl necklace: exchange interactions and zero-field splittings in a C <sub>3</sub> -symmetric Mn <sup>III</sup> <sub>6</sub> complex. Dalton Transactions, 2010, 39, 192-199.	1.6	30
38	Advanced finite-temperature Lanczos method for anisotropic spin systems. European Physical Journal B, 2014, 87, 1.	0.6	26
39	Structurally Flexible and Solution Stable [Ln <sub>4</sub> TM <sub>8</sub> (OH) <sub>8</sub> (L) <sub>8</sub> (O <sub>2</sub> CR) <sub>8</sub> (MeOH) <sub>8</sub> ]·xH <sub>2</sub> O: A Playground for Magnetic Refrigeration. Inorganic Chemistry, 2016, 55, 10535-10546.	2.6	26
40	Efficient implementation of the Lanczos method for magnetic systems. Journal of Computational Physics, 2008, 227, 4512-4517.	1.9	25
41	Suppression of Magnetic Quantum Tunneling in a Chiral Single-Molecule Magnet by Ferromagnetic Interactions. Inorganic Chemistry, 2017, 56, 15119-15129.	1.9	25
42	Heisenberg exchange parameters of molecular magnets from the high-temperature susceptibility expansion. Physical Review B, 2001, 64, .	1.1	24
43	Molecular magnetism. Lecture Notes in Physics, 2004, , 155-194.	0.3	24
44	Theoretical design of molecular nanomagnets for magnetic refrigeration. Applied Physics Letters, 2013, 103, .	1.5	24
45	An [Fe <sup>III</sup> <sub>34</sub> ] Molecular Metal Oxide. Angewandte Chemie - International Edition, 2019, 58, 16903-16906.	7.2	24
46	Tri-, tetra- and octa-metallic vanadium(III) clusters from new, simple starting materials: interplay of exchange and anisotropy effects. Dalton Transactions, 2009, , 9402.	1.6	23
47	Large-scale numerical investigations of the antiferromagnetic Heisenberg icosidodecahedron. Journal of Magnetism and Magnetic Materials, 2013, 327, 103-109.	1.0	22
48	Partition functions and symmetric polynomials. American Journal of Physics, 2002, 70, 53-57.	0.3	21
49	Frustration effects in antiferromagnetic molecules: The cuboctahedron. Polyhedron, 2009, 28, 1620-1623.	1.0	21
50	Thermodynamics of the one-dimensional frustrated Heisenberg ferromagnet with arbitrary spin. Physical Review B, 2011, 84, .	1.1	21
51	Combining Complementary Ligands into one Framework for the Construction of a Ferromagnetically Coupled [Mn <sup>III</sup> <sub>12</sub> ] Wheel. Chemistry - A European Journal, 2014, 20, 3010-3013.	1.7	20
52	Copper Lanthanide Phosphonate Cages: Highly Symmetric {Cu <sub>3</sub> Ln <sub>9</sub> P <sub>6</sub> } and {Cu <sub>6</sub> Ln <sub>6</sub> P <sub>6</sub> } Clusters with C <sub>3v</sub> and D <sub>3h</sub> Symmetry. Inorganic Chemistry, 2015, 54, 6331-6337.	1.9	20
53	Magnon Crystallization in the Kagome Lattice Antiferromagnet. Physical Review Letters, 2020, 125, 117207.	2.9	20
54	Numerical renormalization group calculations of the magnetization of Kondo impurities with and without uniaxial anisotropy. Physical Review B, 2013, 87, .	1.1	19



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73	Fermionic molecular dynamics: Ensembles and fluctuations therein. Nuclear Physics A, 1995, 583, 347-352.	0.6	12
74	Inelastic neutron scattering study and Hubbard model description of the antiferromagnetic tetrahedral molecule Ni <sub>4</sub> Mo <sub>12</sub> . European Physical Journal B, 2010, 73, 515-526.	0.6	12
75	Hydrophobicity-Driven Self-Assembly of an Eighteen-Membered Honeycomb Lattice with Almost Classical Spins. Chemistry - A European Journal, 2016, 22, 14846-14850.	1.7	12
76	Young's moduli of carbon materials investigated by various classical molecular dynamics schemes. Physica E: Low-Dimensional Systems and Nanostructures, 2018, 99, 215-219.	1.3	12
77	Order in disorder: solution and solid-state studies of [M <sub>III</sub> 2M <sub>II</sub> 5] wheels (M <sup>III</sup> = Cr, Al); Tj ETQq1 1 0.784314 rgBT/Overlo	1.6	12
78	Ni <sub>II</sub> <sup>36</sup> -Containing 54-Tungsto-6-Silicate: Synthesis, Structure, Magnetic and Electrochemical Studies. Chemistry - A European Journal, 2021, 27, 15081-15085.	1.7	12
79	Linking [Fe <sub>III</sub> 3] triangles with "double-headed" phenolic oximes. Chemical Communications, 2011, 47, 6018.	2.2	11
80	Phase diagram of the alternating-spin Heisenberg chain with extra isotropic three-body exchange interactions. European Physical Journal B, 2014, 87, 1.	0.6	11
81	Switching from antiferromagnetic to ferromagnetic coupling in heptanuclear [M <sup>t</sup> <sub>6</sub> M <sup>c</sup> ] <sup>n+</sup> complexes by going from an achiral to a chiral triplesalen ligand. Dalton Transactions, 2014, 43, 9690-9703.	1.6	11
82	Classical molecular dynamics investigations of biphenyl-based carbon nanomembranes. Beilstein Journal of Nanotechnology, 2014, 5, 865-871.	1.5	10
83	Magneto-Structural Analysis of Iron(III) Keggin Polyoxometalates. Journal of Physical Chemistry A, 2017, 121, 1310-1318.	1.1	10
84	Periodic thermodynamics of the Rabi model with circular polarization for arbitrary spin quantum numbers. Physical Review E, 2019, 100, 042141.	0.8	10
85	Flat-band physics in the spin-1/2 sawtooth chain. European Physical Journal B, 2020, 93, 1.	0.6	10
86	Exchange interactions and magnetic anisotropy in the Ni <sub>4</sub> ™ magnetic molecule. Phase Transitions, 2005, 78, 47-59.	0.6	9
87	Theoretical estimates for proton-NMR spin-lattice relaxation rates of heterometallic spin rings. Journal of Magnetism and Magnetic Materials, 2006, 302, 206-210.	1.0	9
88	An [Fe <sub>III</sub> 30] molecular metal oxide. Chemical Communications, 2021, 58, 52-55.	2.2	9
89	Systematic Study of the Interaction Between V <sup>IV</sup> Centres and Ln <sup>III</sup> Ions in Well Defined {V <sub>2</sub> IV Ln <sub>III</sub> }{As <sub>III</sub> W <sub>9</sub> O <sub>33</sub> } <sub>2</sub> Sandwich-Type Clusters: Part 2. Journal of Cluster Science, 2013, 24, 979-988.	1.7	8
90	Rational Improvement of Single-Molecule Magnets by Enforcing Ferromagnetic Interactions. Chemistry - A European Journal, 2019, 25, 4992-5004.	1.7	8

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91	Magnetic and electronic properties of the iron-containing polyoxotungstate [Fe <sub>4</sub> (H <sub>2</sub> O) <sub>10</sub> ( $\mu^2$ -SbW <sub>9</sub> O <sub>33</sub> ) <sub>2</sub> ] <sub>6</sub> . Journal of Applied Physics, 2006, 99, 08J505.	1.1	7
92	Alternating-spin $S = 3/2$ and $J = 1/2$ Heisenberg chain with isotropic three-body exchange interactions. European Physical Journal B, 2016, 89, 1.	0.6	7
93	Floquet theory of the analytical solution of a periodically driven two-level system. Applicable Analysis, 2021, 100, 992-1009.	0.6	7
94	Frustration Effects in Magnetic Molecules. Journal of Low Temperature Physics, 2007, 142, 283-288.	0.6	6
95	Local entanglement and string order parameter in dimerized models. Journal of Physics Condensed Matter, 2019, 31, 505602.	0.7	6
96	Decoherence of a singlet-triplet superposition state under dipolar interactions of an uncorrelated environment. Physical Review B, 2020, 101, .	1.1	6
97	Accuracy of the typicality approach using Chebyshev polynomials. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2021, 76, 823-834.	0.7	6
98	Finite-Size Scaling of Typicality-Based Estimates. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2020, 75, 465-473.	0.7	6
99	Frustration-induced exotic properties of magnetic molecules. Comptes Rendus Chimie, 2007, 10, 15-20.	0.2	5
100	Optimization of Single-Molecule Magnets by Suppression of Quantum Tunneling of the Magnetization. European Journal of Inorganic Chemistry, 2020, 2020, 3222-3235.	1.0	5
101	Hendecanuclear [Cu <sub>6</sub> Gd <sub>5</sub> ] magnetic cooler with high molecular symmetry of D <sub>3h</sub> . Chinese Chemical Letters, 2021, 32, 838-841.	4.8	5
102	Observation of phase synchronization and alignment during free induction decay of quantum spins with Heisenberg interactions. New Journal of Physics, 2021, 23, 083038.	1.2	5
103	Frustrated magnetism of spin- $\frac{1}{2}$ Heisenberg diamond and octahedral chains as a statistical mechanical monomer-dimer problem. Physical Review B, 2022, 105, .	1.1	5
104	Exact diagonalization studies of doped Heisenberg spin rings. Journal of Magnetism and Magnetic Materials, 2005, 290-291, 341-344.	1.0	4
105	Solitary waves on finite-size antiferromagnetic quantum Heisenberg spin rings. Journal of Magnetism and Magnetic Materials, 2006, 306, 79-84.	1.0	4
106	An [Fe III 34 ] Molecular Metal Oxide. Angewandte Chemie, 2019, 131, 17059-17062.	1.6	4
107	Supersymmetric spin-phonon coupling prevents odd integer spins from quantum tunneling. European Physical Journal B, 2021, 94, 1.	0.6	4
108	Theoretical formation of carbon nanomembranes under realistic conditions using classical molecular dynamics. Physical Review B, 2021, 103, .	1.1	4





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127	Thermal density matrix renormalization group for highly frustrated quantum spin chains: A user perspective. <i>Journal of Magnetism and Magnetic Materials</i> , 2019, 487, 165327.	1.0	1
128	Stochastic thermodynamics of a finite quantum system coupled to a heat bath. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2021, 76, 731-745.	0.7	1
129	Investigation of electron-induced cross-linking of self-assembled monolayers by scanning tunneling microscopy. <i>Beilstein Journal of Nanotechnology</i> , 0, 13, 462-471.	1.5	1
130	Revisiting and modeling the magnetism of hole-doped spin chains in. <i>Journal of Magnetism and Magnetic Materials</i> , 2007, 310, e397-e399.	1.0	0
131	Phase diagrams of Heisenberg chains with different cell spins: role of the tree-site exchange interactions. <i>Journal of Physics: Conference Series</i> , 2019, 1186, 012014.	0.3	0
132	ROTATIONAL BAND STRUCTURE OF LOW-LYING EXCITATIONS IN SMALL HEISENBERG SYSTEMS. , 2002, , .		0
133	Isothermal Molecular Dynamics in Classical and Quantum Mechanics. , 2004, , 111-124.		0
134	Evaluation of Magnetic Spectra Using the Irreducible Tensor Operator Approach. , 2010, , 575-588.		0
135	Fermionic Molecular Dynamics: Multifragmentation in Heavy-Ion Collisions and in Excited Nuclei. , 1997, , 83-90.		0
136	Liquid-Gas Phase Transition in Finite Nuclei within Fermionic Molecular Dynamics. , 1999, , 411-420.		0