

Paolo Santini

List of Publications by Year in descending order

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141
papers

5,531
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71102

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70
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144
all docs

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docs citations

144
times ranked

3323
citing authors

#	ARTICLE	IF	CITATIONS
1	Multipolar interactions in f -electron systems: The paradigm of actinide dioxides. <i>Reviews of Modern Physics</i> , 2009, 81, 807-863.	45.6	386
2	Engineering the coupling between molecular spin qubits by coordination chemistry. <i>Nature Nanotechnology</i> , 2009, 4, 173-178.	31.5	374
3	Molecular Engineering of Antiferromagnetic Rings for Quantum Computation. <i>Physical Review Letters</i> , 2005, 94, 207208.	7.8	291
4	Crystal Field Model of the Magnetic Properties of URu ₂ Si ₂ . <i>Physical Review Letters</i> , 1994, 73, 1027-1030.	7.8	206
5	A modular design of molecular qubits to implement universal quantum gates. <i>Nature Communications</i> , 2016, 7, 11377.	12.8	196
6	Triple- q -Octupolar Ordering in NpO ₂ . <i>Physical Review Letters</i> , 2002, 89, 187202.	7.8	168
7	Magnetism of actinide compounds. <i>Advances in Physics</i> , 1999, 48, 537-653.	14.4	142
8	Magnetic-Octupole Order in Neptunium Dioxide?. <i>Physical Review Letters</i> , 2000, 85, 2188-2191.	7.8	115
9	Proposal for Quantum Gates in Permanently Coupled Antiferromagnetic Spin Rings without Need of Local Fields. <i>Physical Review Letters</i> , 2005, 94, 190501.	7.8	115
10	Spin dynamics of molecular nanomagnets unravelled at atomic scale by four-dimensional inelastic neutron scattering. <i>Nature Physics</i> , 2012, 8, 906-911.	16.7	108
11	Magnetic excitations and dynamical Jahn-Teller distortions in UO ₂ . <i>Physical Review B</i> , 1999, 59, 13892-13900.	3.2	102
12	Single molecule magnets for quantum computation. <i>Journal Physics D: Applied Physics</i> , 2007, 40, 2999-3004.	2.8	102
13	Entanglement in Supramolecular Spin Systems of Two Weakly Coupled Antiferromagnetic Rings (Purple- T_j ETQq1 1 0.784314 rgBT / Overlap). <i>Physical Review Letters</i> , 2010, 104, 037203.	7.8	99
14	Quantum Oscillations of the Total Spin in a Heterometallic Antiferromagnetic Ring: Evidence from Neutron Spectroscopy. <i>Physical Review Letters</i> , 2007, 98, 167401.	7.8	97
15	Understanding magnetic relaxation in single-ion magnets with high blocking temperature. <i>Physical Review B</i> , 2020, 101, .	3.2	94
16	Spin dynamics of heterometallic Cr ₇ M wheels (M=Mn, Zn, Ni) probed by inelastic neutron scattering. <i>Physical Review B</i> , 2005, 71, .	3.2	89
17	Quantum hardware simulating four-dimensional inelastic neutron scattering. <i>Nature Physics</i> , 2019, 15, 455-459.	16.7	89
18	Molecular Nanomagnets as Quantum Simulators. <i>Physical Review Letters</i> , 2011, 107, 230502.	7.8	79

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19	SMixing and Quantum Tunneling of the Magnetization in Molecular Nanomagnets. Physical Review Letters, 2004, 92, 207205.	7.8	77
20	Spin triangles as optimal units for molecule-based quantum gates. Physical Review B, 2007, 76, .	3.2	67
21	Breakdown of the Giant Spin Model in the Magnetic Relaxation of the Mn ₆ Nanomagnets. Physical Review Letters, 2008, 100, 157203.	7.8	67
22	NMR as a Probe of the Relaxation of the Magnetization in Magnetic Molecules. Physical Review Letters, 2005, 94, 077203.	7.8	66
23	Molecular routes for spin cluster qubits. Dalton Transactions, 2006, , 2810.	3.3	66
24	Topology and spin dynamics in magnetic molecules. Physical Review B, 2005, 72, .	3.2	61
25	Switchable Interaction in Molecular Double Qubits. Chem, 2016, 1, 727-752.	11.7	60
26	Molecular nanomagnets with switchable coupling for quantum simulation. Scientific Reports, 2014, 4, 7423.	3.3	58
27	Hidden Order and Low-Energy Excitations in NpO ₂ . Physical Review Letters, 2006, 97, 207203.	7.8	57
28	Dynamics of extensively reconstructed surfaces: Si(111) 2 \times 1. Physical Review Letters, 1989, 62, 3070-3073.	7.8	55
29	High-Temperature Slow Relaxation of the Magnetization in Ni ₁₀ Magnetic Molecules. Physical Review Letters, 2006, 97, 207201.	7.8	54
30	Behavior of URu ₂ Si ₂ in an applied magnetic field. Physical Review B, 1998, 57, 5191-5199.	3.2	50
31	Successful grafting of isolated molecular Cr^{3+} on Au(111) surface. Physical Review B, 2009, 79, .	3.2	49
32	Multipolar ordering in NpO ₂ below 25 K. Journal of Physics Condensed Matter, 2003, 15, S2287-S2296.	1.8	48
33	Perturbative approach to mixing inf-electron systems: Application to actinide dioxides. Physical Review B, 2005, 71, .	3.2	48
34	Portraying entanglement between molecular qubits with four-dimensional inelastic neutron scattering. Nature Communications, 2017, 8, 14543.	12.8	48
35	Molecular Nanomagnets as Qubits with Embedded Quantum-Error Correction. Journal of Physical Chemistry Letters, 2020, 11, 8610-8615.	4.6	48
36	Dynamics and structural assessment of open semiconductor surfaces: GaAs(110). Physical Review B, 1990, 42, 11942-11945.	3.2	46

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37	Multipolar, magnetic, and vibrational lattice dynamics in the low-temperature phase of uranium dioxide. <i>Physical Review B</i> , 2011, 84, .	3.2	44
38	Unveiling phonons in a molecular qubit with four-dimensional inelastic neutron scattering and density functional theory. <i>Nature Communications</i> , 2020, 11, 1751.	12.8	43
39	Quantum Magneto-Oscillations in a Supramolecular Mn(II)-[3Å–3] Grid. <i>Physical Review Letters</i> , 2004, 92, 096403.	7.8	42
40	Spin dynamics and tunneling of the Néel vector in the Fe ₁₀ magnetic wheel. <i>Physical Review B</i> , 2005, 71, .	3.2	41
41	Many-Body Models for Molecular Nanomagnets. <i>Physical Review Letters</i> , 2013, 110, 157204.	7.8	41
42	Evidence of spin singlet ground state in the frustrated antiferromagnetic ring Cr_8 . <i>Physical Review B</i> , 2009, 79, .	3.2	39
43	Inelastic neutron scattering study of the multipolar order parameter in NpO_2 . <i>Physical Review B</i> , 2008, 78, .	3.2	37
44	Resonant x-ray scattering study of magnetic-dipole and electric-quadrupole order in $\text{U}_0.75\text{Np}_0.25\text{O}_2$. <i>Physical Review B</i> , 2004, 70, .	3.2	36
45	A Cost-Effective Semi-Ab Initio Approach to Model Relaxation in Rare-Earth Single-Molecule Magnets. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 8826-8832.	4.6	35
46	Quadrupolar Waves in Uranium Dioxide. <i>Physical Review Letters</i> , 2010, 105, 167201.	7.8	34
47	Magnetic Exchange Interactions in the Molecular Nanomagnet Mn_{12} . <i>Physical Review Letters</i> , 2017, 119, 217202.	7.8	34
48	Inelastic neutron scattering study of the molecular grid nanomagnet Mn-[3Å–3]. <i>Physical Review B</i> , 2004, 69, .	3.2	33
49	Spherical neutron spin polarimetry of anisotropic magnetic fluctuations in UO_2 . <i>Physical Review B</i> , 2005, 72, .	3.2	33
50	Localized 4f States and Dynamic Jahn-Teller Effect in PrO_2 . <i>Physical Review Letters</i> , 2001, 86, 2082-2085.	7.8	32
51	Direct observation of finite size effects in chains of antiferromagnetically coupled spins. <i>Nature Communications</i> , 2015, 6, 7061.	12.8	30
52	Surface phonon dispersion curves in GaAs(110) and Ge(111)2 Å–1: a critical comparison. <i>Surface Science</i> , 1991, 241, 346-352.	1.9	29
53	Magnetic Anisotropy of Cr_7Ni Spin Clusters on Surfaces. <i>Advanced Functional Materials</i> , 2012, 22, 3706-3713.	14.9	28
54	Quantum Information Processing with Hybrid Spin-Photon Qubit Encoding. <i>Physical Review Letters</i> , 2013, 111, 110501.	7.8	28

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55	Intra- and inter-multiplet magnetic excitations in a tetrairon(III) molecular cluster. <i>Physical Review B</i> , 2004, 70, .	3.2	27
56	Studies of a Large Odd-Numbered Electron Metal Ring: Inelastic Neutron Scattering and Muon Spin Relaxation Spectroscopy of Cr_8Mn . <i>Chemistry - A European Journal</i> , 2016, 22, 1779-1788.	3.3	27
57	A Detailed Study of the Magnetism of Chiral $\{\text{Cr}_7\text{M}\}$ Rings: An Investigation into Parametrization and Transferability of Parameters. <i>Journal of the American Chemical Society</i> , 2014, 136, 9763-9772.	13.7	26
58	$[\text{CrF}(\text{O})_2\text{C}(\text{sup}i\text{t})\text{Bu}]_9$: Synthesis and Characterization of a Regular Homometallic Ring with an Odd Number of Metal Centers and Electrons. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 8856-8859.	13.8	26
59	Field-Dependent Energy Scales in URu_2Si_2 . <i>Physical Review Letters</i> , 2000, 85, 654-657.	7.8	25
60	Digital quantum simulators in a scalable architecture of hybrid spin-photon qubits. <i>Scientific Reports</i> , 2015, 5, 16036.	3.3	25
61	Assessing the Nature of Chiral-Induced Spin Selectivity by Magnetic Resonance. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 6341-6347.	4.6	25
62	Finite-size-scaling study of the gap formation in the $\tilde{\text{Kondo-necklace}}$ model. <i>Physical Review B</i> , 1992, 46, 7422-7426.	3.2	24
63	Non-Dipolar Degrees of Freedom in Neptunium Dioxide. <i>Journal of the Physical Society of Japan</i> , 2002, 71, 11-16.	1.6	24
64	Theoretical design of molecular nanomagnets for magnetic refrigeration. <i>Applied Physics Letters</i> , 2013, 103, .	3.3	24
65	Intrinsic and extrinsic effects in surfaces: Acoustic-phonon softening of capped Si(111) surfaces. <i>Physical Review B</i> , 1992, 46, 9865-9868.	3.2	22
66	Octupolar order in $\text{Ce}_3\text{B}_2\text{O}_7$: A specific heat investigation. <i>Physica B: Condensed Matter</i> , 2005, 359-361, 1087-1089.	2.7	22
67	Elementary excitations in antiferromagnetic Heisenberg spin segments. <i>Physical Review B</i> , 2007, 76, .	3.2	22
68	Inelastic neutron scattering investigations of molecular nanomagnets. <i>Inorganica Chimica Acta</i> , 2008, 361, 3771-3776.	2.4	22
69	Exchange interactions in $\text{Ca}_3\text{Co}_2\text{O}_7$. <i>Physical Review B</i> , 2007, 76, 040407.	3.2	22
70	Crystal-field potentials of PrFe_2Si_2 and PrFe_2Ge_2 as deduced from inelastic neutron scattering and specific heat measurements. <i>Journal of Physics Condensed Matter</i> , 1995, 7, 8317-8330.	1.8	21
71	Inelastic neutron scattering and frequency-domain magnetic resonance studies of $S=4$ and $S=12$ Mn single-molecule magnets. <i>Physical Review B</i> , 2010, 81, .	3.2	21
72	Anisotropy of CoII transferred to the Cr_7Co polymetallic cluster <i>via</i> strong exchange interactions. <i>Chemical Science</i> , 2018, 9, 3555-3562.	7.4	20

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73	Counteracting dephasing in Molecular Nanomagnets by optimized qudit encodings. Npj Quantum Information, 2021, 7, .	6.7	20
74	Macroscopic evidence of quantum coherent oscillations of the total spin in the Mn- $[Mn_3]$ molecular nanomagnet. European Physical Journal B, 2003, 36, 169-173.	1.5	19
75	X-ray magnetic circular dichroism investigation of spin and orbital moments in Cr ₈ and Cr ₇ antiferromagnetic rings. Physical Review B, 2008, 77, .	3.2	19
76	Rotational bands in open antiferromagnetic rings: A neutron spectroscopy study of Cr ₈ Zn. Physical Review B, 2009, 79, .	3.2	19
77	Relaxation dynamics in the frustrated Cr_9 ring probed by NMR. Physical Review B, 2016, 93, .	3.2	15
78	Anisotropic magnetic fluctuations in 3- antiferromagnets. Journal of Magnetism and Magnetic Materials, 2007, 310, 1698-1702.	2.3	18
79	Varying spin state composition by the choice of capping ligand in a family of molecular chains: detailed analysis of magnetic properties of chromium(III) horseshoes. Dalton Transactions, 2011, 40, 2725.	3.3	18
80	Santini and Amoretti Reply:. Physical Review Letters, 1995, 74, 4098-4098.	7.8	16
81	Magnetic correlations in the Anderson lattice: An exact-diagonalization study. Physical Review B, 1993, 47, 1130-1133.	3.2	15
82	Λ scaling in random walks with fluctuating variance. Physical Review E, 2000, 61, 93-99.	2.1	15
83	Probing local magnetization in molecular heterometallic Cr_2 . Physical Review B, 2010, 82, .	3.2	15
84	Relaxation dynamics in a Fe Cr_7 nanomagnet. Physical Review B, 2013, 87, .	3.2	15
85	Many-body <i>ab initio</i> study of antiferromagnetic Cr_7M rings. Physical Review B, 2016, 94, .	3.2	15
86	Embedded quantum-error correction and controlled-phase gate for molecular spin qubits. AIP Advances, 2021, 11, .	1.3	15
87	Phonon-induced relaxation in the giant keplerate molecule $Mo_{72}Fe_{30}$. Physical Review B, 2010, 82, .	3.2	14
88	Phonon-induced relaxation in the Cr_7 molecule probed by NMR. Physical Review B, 2010, 82, .	3.2	14
89	Magnetic properties and relaxation dynamics of a frustrated Ni ₇ molecular nanomagnet. Journal of Physics Condensed Matter, 2012, 24, 104006.	1.8	14
90	Superadiabatic driving of a three-level quantum system. Physical Review A, 2017, 96, .	2.5	14

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91	Simulating Static and Dynamic Properties of Magnetic Molecules with Prototype Quantum Computers. <i>Magnetochemistry</i> , 2021, 7, 117.	2.4	14
92	Crystal-field excitations and gap opening in Tm: YBa ₂ Cu ₄ O ₈ by inelastic neutron scattering. <i>Physica C: Superconductivity and Its Applications</i> , 1994, 221, 227-236.	1.2	13
93	Inelastic-neutron-scattering study of excited spin multiplets and low-energy phonons in the Fe ₈ nanomagnet: Implications for relaxation. <i>Physical Review B</i> , 2006, 73, .	3.2	13
94	Quantum error correction with molecular spin qubits. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 20030-20039.	2.8	13
95	Magnetic properties and chiral states of a trimetallic uranium complex. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 486001.	1.8	12
96	First-principles many-body models for electron transport through molecular nanomagnets. <i>Physical Review B</i> , 2019, 99, .	3.2	12
97	Magnetization and susceptibility of the Kondo compounds $x=0, 1, 1.5, 2$. <i>Journal of Physics Condensed Matter</i> , 1998, 10, 4465-4475.	1.8	11
98	Robustness of quantum gates with hybrid spin-photon qubits in superconducting resonators. <i>Physical Review A</i> , 2014, 89, .	2.5	11
99	Supramolecular Complexes for Quantum Simulation. <i>Magnetochemistry</i> , 2016, 2, 37.	2.4	11
100	Unravelling the Spin Dynamics of Molecular Nanomagnets with Four-Dimensional Inelastic Neutron Scattering. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 1106-1118.	2.0	11
101	Neutron spectroscopy and magnetic relaxation of the Mn ₆ nanomagnets. <i>Polyhedron</i> , 2009, 28, 1940-1944.	2.2	10
102	[CrF(O ₂) ₂ CBu ₂] ₉ : Synthesis and Characterization of a Regular Homometallic Ring with an Odd Number of Metal Centers and Electrons. <i>Angewandte Chemie</i> , 2016, 128, 9002-9005.	2.0	10
103	Constructing clock-transition-based two-qubit gates from dimers of molecular nanomagnets. <i>Physical Review Research</i> , 2020, 2, .	3.6	10
104	Spin Dynamics in Hybrid Iron Oxide-Gold Nanostructures. <i>Journal of Physical Chemistry C</i> , 2015, 119, 1224-1233.	3.1	9
105	Self-consistent crystal-field description of tetragonal Pr and U compounds with Van Vleck induced magnetism. <i>Journal of Applied Physics</i> , 1993, 73, 6560-6562.	2.5	8
106	Classical fluctuations and anisotropy in quasi-one-dimensional antiferromagnets. <i>Physical Review B</i> , 1996, 54, 6327-6332.	3.2	8
107	AF molecular rings for quantum computation. <i>Polyhedron</i> , 2005, 24, 2562-2567.	2.2	8
108	Molecular spin clusters for quantum computation. <i>Journal of Magnetism and Magnetic Materials</i> , 2007, 310, e501-e502.	2.3	8

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109	Unconventional Nonequilibrium Dynamics in $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle \text{Ni} \langle \text{mml:mi} \rangle \langle \text{mml:mn} \rangle 10 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:math} \rangle \text{Magnetic Molecules: Evidence from NMR. Physical Review Letters, 2009, 102, 177201.}$	7.8	8
110	Analysis of the crystal field level splittings for Tm ³⁺ in YBCO-type compounds. Physica B: Condensed Matter, 1994, 193, 221-231.	2.7	7
111	Molecular-field theory of moment reduction in Kondo systems with crystal-field effects. Zeitschrift für Physik B-Condensed Matter, 1996, 100, 95-104.	1.1	7
112	Spin dynamics of Fe ₇ M (M=Zn,Mn) heterometallic rings probed by neutron spectroscopy. Physical Review B, 2007, 75, .	3.2	7
113	Neutron spectroscopy and anisotropy of the magnetic properties of UOS: Interpretation in a crystal-field and molecular-field model. Journal of Magnetism and Magnetic Materials, 1995, 139, 339-346.	2.3	7
114	Polarized neutron scattering study of the magnetic response across TN in a single crystal of UO ₂ . Journal of Applied Physics, 1999, 85, 4524-4526.	2.5	6
115	Unified crystal-field picture for actinide dioxides. Journal of Physics and Chemistry of Solids, 2007, 68, 2020-2023.	4.0	6
116	Detection of entanglement between collective spins. Physical Review B, 2013, 88, .	3.2	6
117	Long-lasting hybrid quantum information processing in a cavity-protection regime. Physical Review B, 2016, 93, .	3.2	6
118	Competition between Kondo effect and magnetic interaction in Kondo systems. Physica B: Condensed Matter, 1997, 230-232, 523-528.	2.7	4
119	Quantum fluctuations of the total spin in molecular nanomagnets: Evidence from torque and specific heat. Journal of Applied Physics, 2004, 95, 7348-7350.	2.5	4
120	Magnetization and spin dynamics of a Cr-based magnetic cluster. Journal of Magnetism and Magnetic Materials, 2010, 322, 1262-1264.	2.3	4
121	Correlation effects on electronic and optical properties of a C ₆₀ molecule: A variational Monte Carlo study. Physical Review B, 1996, 54, 13611-13615.	3.2	3
122	Quantum fluctuations and anisotropy in quasi-one-dimensional antiferromagnets. Physical Review B, 1997, 56, 5373-5379.	3.2	3
123	Temperature dependence of single particle excitations in a S=1 chain: Exact diagonalization calculations compared to neutron scattering experiments. Physical Review B, 2002, 66, .	3.2	3
124	Spin dynamics of molecular nanomagnets. Physica B: Condensed Matter, 2006, 385-386, 301-306.	2.7	3
125	Decay of time-correlations of microscopic observables in magnetic molecules. Physica B: Condensed Matter, 2006, 374-375, 109-113.	2.7	3
126	Relaxation of the magnetization in a molecule containing ions. Journal of Magnetism and Magnetic Materials, 2007, 310, 1450-1451.	2.3	3

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127	Response to "Comment on "Theoretical design of molecular nanomagnets for magnetic refrigeration" [Appl. Phys. Lett. 105, 046101 (2014)]. Applied Physics Letters, 2014, 105, 046102.	3.3	3
128	Relaxation of the magnetization in magnetic molecules. Journal of Applied Physics, 2006, 99, 08D101.	2.5	2
129	Slow magnetic dynamics in the Ni10 family of compounds. Solid State Sciences, 2009, 11, 778-785.	3.2	2
130	Kondo reduction of magnetic moment under high external field in CeCu5: Theoretical interpretation. Solid State Communications, 1997, 103, 585-589.	1.9	1
131	Quantum tunneling of the magnetization in molecular nanomagnets: The crucial role of S mixing. Polyhedron, 2005, 24, 2459-2463.	2.2	1
132	Relaxation dynamics of the Fe8 molecular nanomagnet as probed by nuclear magnetic resonance. Dalton Transactions, 2010, 39, 4869.	3.3	1
133	Surface lattice dynamics of the Pandey-reconstructed Si(111)-2 \times 1: No pathologies in the experimental findings. Surface Science, 1989, 211-212, 335-342.	1.9	0
134	Surface Phonons in Si(111) 2 \times 1: Folding and Chain Effects of the Reconstruction. Physica Scripta, 1989, T25, 305-308.	2.5	0
135	Lattice dynamics of GaAs(110) and Ge(111): 2 \times 1. Vacuum, 1990, 41, 605-607.	3.5	0
136	Spin correlations in dense Kondo systems. Journal of Applied Physics, 1993, 73, 5403-5405.	2.5	0
137	Numerical calculation of correlation functions by boundary condition averaging: test on the one-dimensional Hubbard model. Computer Physics Communications, 1995, 92, 16-20.	7.5	0
138	Moment reduction in Kondo systems with crystal field effects: molecular field theory. Physica B: Condensed Matter, 1995, 206-207, 138-140.	2.7	0
139	Quadrupolar model of the 17.5 K phase transition in URu2Si2. Physica B: Condensed Matter, 1995, 206-207, 421-423.	2.7	0
140	Elementary excitations in uranium dioxide: Unravelling the tangle. Comptes Rendus Physique, 2014, 15, 573-579.	0.9	0
141	Efficient Quantum Simulation of Dynamic Correlations on Superconducting Quantum Computers. , 2019, , .		0