

Liviu Ungur

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

122
papers

15,338
citations

61
h-index

123
g-index

131
ext. papers

17,007
ext. citations

8.1
avg, IF

6.65
L-index

#	Paper	IF	Citations
122	Toroidal centripetal arrangement of the magnetic moment in a Dy ₄ tetrahedron.. <i>Chemical Communications</i> , 2022 ,	5.8	3
121	The Role of Radical Bridges in Polynuclear Single-Molecule Magnets.. <i>Chemistry - A European Journal</i> , 2022 , e202200227	4.8	0
120	Carbonate-free CoAl layered double hydroxides supercapacitors: Controlled precipitation via acid mediated decomplexation. <i>Applied Clay Science</i> , 2022 , 224, 106519	5.2	0
119	Magnetization Dynamics on Isotope-Isomorphous Holmium Single-Molecule Magnets. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 27282	16.4	0
118	A Family of Lanthanide Hydroxo Carboxylates with 1D Polymeric Topology and Ln Butterfly Core Exhibits Switchable Supramolecular Arrangement. <i>Inorganic Chemistry</i> , 2021 , 60, 8049-8061	5.1	6
117	Multiresponsive Spin Crossover Driven by Rotation of Tetraphenylborate Anion in an Iron(III) Complex. <i>CCS Chemistry</i> , 2021 , 3, 453-459	7.2	2
116	Understanding the magnetization blocking mechanism in N-radical-bridged lanthanide single-molecule magnets. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 10303-10310	3.6	6
115	Exploring vibronic coupling in the benzene radical cation and anion with different levels of the GW approximation. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 19054-19070	3.6	0
114	Design of Fe ^{III} Ni ^{III} binuclear complexes using compartmental ligands: synthesis, crystal structures, magnetic properties, and ab initio analysis. <i>Journal of Materials Chemistry C</i> , 2021 , 9, 10912-10926	7.1	3
113	Towards understanding the magnetism of Os(IV) complexes: an insight. <i>Dalton Transactions</i> , 2021 , 50, 12537-12546	4.3	0
112	An Inconspicuous Six-Coordinate Neutral Dy Single-Ion Magnet with Remarkable Magnetic Anisotropy and Stability. <i>Inorganic Chemistry</i> , 2020 , 59, 7158-7166	5.1	18
111	Highly Oxidized States of Phthalocyaninato Terbium(III) Multiple-Decker Complexes Showing Structural Deformations, Biradical Properties and Decreases in Magnetic Anisotropy. <i>Chemistry - A European Journal</i> , 2020 , 26, 8621-8630	4.8	10
110	Modern quantum chemistry with [Open]Molcas. <i>Journal of Chemical Physics</i> , 2020 , 152, 214117	3.9	106
109	Coexistence of Spin-Lattice Relaxation and Phonon-Bottleneck Processes in Gd -Phthalocyaninato Triple-Decker Complexes under Highly Diluted Conditions. <i>Chemistry - A European Journal</i> , 2020 , 26, 8076-8082	4.8	6
108	Magnetic Anisotropy in Divalent Lanthanide Compounds. <i>Angewandte Chemie</i> , 2020 , 132, 12820-12824	3.6	3
107	Single-Molecule Toroidal Design through Magnetic Exchange Coupling. <i>Matter</i> , 2020 , 2, 1481-1493	12.7	16
106	Magnetic Anisotropy in Divalent Lanthanide Compounds. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 12720-12724	16.4	13

105	Deriving the vibronic coupling constants of the cyclopentadienyl radical with density functional theory and GW.. <i>Journal of Chemical Physics</i> , 2020 , 153, 064303	3.9	2
104	Comparison of two field-induced Er single ion magnets. <i>Dalton Transactions</i> , 2019 , 48, 15679-15686	4.3	5
103	OpenMolcas: From Source Code to Insight. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 5925-5964	3.0	310
102	Single Crystal Investigations Unravel the Magnetic Anisotropy of the "Square-In Square" CrDy SMM Coordination Cluster. <i>Frontiers in Chemistry</i> , 2019 , 7, 6	5	8
101	Determination of the electronic structure of a dinuclear dysprosium single molecule magnet without symmetry idealization. <i>Chemical Science</i> , 2019 , 10, 2101-2110	9.4	35
100	Exchange Interactions Switch Tunneling: A Comparative Experimental and Theoretical Study on Relaxation Dynamics by Targeted Metal Ion Replacement. <i>Chemistry - A European Journal</i> , 2018 , 24, 9928-9939	4.8	14
99	Magnetization Blocking in Fe Dy Molecular Magnets: Ab Initio Calculations and EPR Spectroscopy. <i>Chemistry - A European Journal</i> , 2018 , 24, 16652-16661	4.8	13
98	Introduction to the electronic structure, luminescence, and magnetism of lanthanides 2018 , 1-58		6
97	Exchange coupling and single molecule magnetism in redox-active tetraoxolene-bridged dilanthanide complexes. <i>Chemical Science</i> , 2018 , 9, 1221-1230	9.4	49
96	J -pseudospin states and the crystal field of cubic systems. <i>Physical Review B</i> , 2018 , 98,	3.3	4
95	Gold-Catalyzed Post-Ugi Ipso-Cyclization with Switchable Diastereoselectivity. <i>Journal of Organic Chemistry</i> , 2018 , 83, 8170-8182	4.2	26
94	Pursuit of Record Breaking Energy Barriers: A Study of Magnetic Axiality in Diamide Ligated Dy Single-Molecule Magnets. <i>Journal of the American Chemical Society</i> , 2017 , 139, 1420-1423	16.4	149
93	Dynamic Magnetic and Optical Insight into a High Performance Pentagonal Bipyramidal Dy Single-Ion Magnet. <i>Chemistry - A European Journal</i> , 2017 , 23, 5708-5715	4.8	79
92	Dynamic Magnetic and Optical Insight into a High-Performance Pentagonal Bipyramidal DyIII Single-Ion Magnet. <i>Chemistry - A European Journal</i> , 2017 , 23, 5630-5630	4.8	4
91	Ab Initio Crystal Field for Lanthanides. <i>Chemistry - A European Journal</i> , 2017 , 23, 3708-3718	4.8	163
90	Zeeman interaction and Jahn-Teller effect in the \mathbb{B} multiplet. <i>Physical Review B</i> , 2017 , 96,	3.3	10
89	Strong ferromagnetic exchange coupling in a {Ni} cluster mediated through an air-stable tetrazine-based radical anion. <i>Chemical Communications</i> , 2017 , 53, 8660-8663	5.8	33
88	Cycloheptatrienyl trianion: an elusive bridge in the search of exchange coupled dinuclear organolanthanide single-molecule magnets. <i>Chemical Science</i> , 2017 , 8, 231-240	9.4	44

87	The active site of low-temperature methane hydroxylation in iron-containing zeolites. <i>Nature</i> , 2016 , 536, 317-21	50.4	229
86	Giant exchange interaction in mixed lanthanides. <i>Scientific Reports</i> , 2016 , 6, 24046	4.9	38
85	Synthesis, Crystal Structures, Magnetic Properties, and Theoretical Investigation of a New Series of Ni-Ln-W Heterotrimetallics: Understanding the SMM Behavior of Mixed Polynuclear Complexes. <i>Inorganic Chemistry</i> , 2016 , 55, 12158-12171	5.1	35
84	Probing the structural and magnetic properties of a new family of centrosymmetric dinuclear lanthanide complexes. <i>RSC Advances</i> , 2016 , 6, 56668-56673	3.7	8
83	Multitechnique investigation of Dy - implications for coupled lanthanide clusters. <i>Chemical Science</i> , 2016 , 7, 4347-4354	9.4	60
82	Symmetry-Supported Magnetic Blocking at 20 K in Pentagonal Bipyramidal Dy(III) Single-Ion Magnets. <i>Journal of the American Chemical Society</i> , 2016 , 138, 2829-37	16.4	601
81	Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. <i>Journal of Computational Chemistry</i> , 2016 , 37, 506-41	3.5	1047
80	A Stable Pentagonal Bipyramidal Dy(III) Single-Ion Magnet with a Record Magnetization Reversal Barrier over 1000 K. <i>Journal of the American Chemical Society</i> , 2016 , 138, 5441-50	16.4	738
79	Strategies toward High-Temperature Lanthanide-Based Single-Molecule Magnets. <i>Inorganic Chemistry</i> , 2016 , 55, 10043-10056	5.1	248
78	Tetraanionic biphenyl lanthanide complexes as single-molecule magnets. <i>Inorganic Chemistry</i> , 2015 , 54, 2374-82	5.1	41
77	Influencing the properties of dysprosium single-molecule magnets with phosphorus donor ligands. <i>Nature Communications</i> , 2015 , 6, 7492	17.4	112
76	Heterometallic 3d-4f single-molecule magnets: ligand and metal ion influences on the magnetic relaxation. <i>Inorganic Chemistry</i> , 2015 , 54, 3631-42	5.1	81
75	Tuning the Magnetic Interactions and Relaxation Dynamics of Dy ₂ Single-Molecule Magnets. <i>Chemistry - A European Journal</i> , 2015 , 21, 14099-106	4.8	79
74	Observation of unusual slow-relaxation of the magnetisation in a Gd-EDTA chelate. <i>Dalton Transactions</i> , 2015 , 44, 20321-5	4.3	50
73	Desolvation-Driven 100-Fold Slow-down of Tunneling Relaxation Rate in Co(II)-Dy(III) Single-Molecule Magnets through a Single-Crystal-to-Single-Crystal Process. <i>Scientific Reports</i> , 2015 , 5, 16621	4.9	78
72	Magnetic Relaxation in Single-Electron Single-Ion Cerium(III) Magnets: Insights from Ab Initio Calculations. <i>Chemistry - A European Journal</i> , 2015 , 21, 13812-9	4.8	50
71	Computational Modelling of the Magnetic Properties of Lanthanide Compounds 2015 , 153-184		17
70	An NCN-pincer ligand dysprosium single-ion magnet showing magnetic relaxation via the second excited state. <i>Scientific Reports</i> , 2014 , 4, 5471	4.9	129

69	A Catalyst with Two-Coordinate Nickel: Theoretical and Catalytic Studies. <i>European Journal of Inorganic Chemistry</i> , 2014 , 2014, 818-823	2.3	47
68	Fine-tuning the local symmetry to attain record blocking temperature and magnetic remanence in a single-ion magnet. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 4413-7	16.4	327
67	Single-molecule magnetism in a family of {Co(III)2Dy(III)2} butterfly complexes: effects of ligand replacement on the dynamics of magnetic relaxation. <i>Inorganic Chemistry</i> , 2014 , 53, 4303-15	5.1	78
66	Stabilization of a cobalt-cobalt bond by two cyclic alkyl amino carbenes. <i>Journal of the American Chemical Society</i> , 2014 , 136, 1770-3	16.4	50
65	Coupling strategies to enhance single-molecule magnet properties of erbium-cyclooctatetraenyl complexes. <i>Journal of the American Chemical Society</i> , 2014 , 136, 8003-10	16.4	236
64	Spectroscopic determination of crystal field splittings in lanthanide double deckers. <i>Chemical Science</i> , 2014 , 5, 3287	9.4	101
63	Field-induced multiple relaxation mechanism of Co(III)2Dy(III) compound with the dysprosium ion in a low-symmetrical environment. <i>Inorganic Chemistry</i> , 2014 , 53, 12658-63	5.1	39
62	Chemical tuning of the magnetic relaxation in dysprosium(iii) mononuclear complexes. <i>Dalton Transactions</i> , 2014 , 43, 12146-9	4.3	44
61	Single-molecule toroics in Ising-type lanthanide molecular clusters. <i>Chemical Society Reviews</i> , 2014 , 43, 6894-905	58.5	278
60	Modifying the properties of 4f single-ion magnets by peripheral ligand functionalisation. <i>Chemical Science</i> , 2014 , 5, 1650-1660	9.4	144
59	Electronic structure and slow magnetic relaxation of low-coordinate cyclic alkyl(amino) carbene stabilized iron(I) complexes. <i>Journal of the American Chemical Society</i> , 2014 , 136, 11964-71	16.4	122
58	Correction to "Key Role of Frustration in Suppression of Magnetization Blocking in Single-Molecule Magnets". <i>Journal of Physical Chemistry Letters</i> , 2014 , 5, 1678	6.4	2
57	A heterometallic Fe(II)-Dy(III) single-molecule magnet with a record anisotropy barrier. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 12966-70	16.4	207
56	Fine-tuning the Local Symmetry to Attain Record Blocking Temperature and Magnetic Remanence in a Single-Ion Magnet. <i>Angewandte Chemie</i> , 2014 , 126, 4502-4506	3.6	67
55	Ein heterometallischer FeII-DyIII-Einzelmolekülmagnet mit Rekord-Anisotropiebarriere. <i>Angewandte Chemie</i> , 2014 , 126, 13180-13184	3.6	30
54	Magnetic relaxation pathways in lanthanide single-molecule magnets. <i>Nature Chemistry</i> , 2013 , 5, 673-8	17.6	583
53	Switching the anisotropy barrier of a single-ion magnet by symmetry change from quasi-D5h to quasi-Oh. <i>Chemical Science</i> , 2013 , 4, 3310	9.4	402
52	Key Role of Frustration in Suppression of Magnetization Blocking in Single-Molecule Magnets. <i>Journal of Physical Chemistry Letters</i> , 2013 , 4, 3565-3569	6.4	55

51	Angular-resolved magnetometry beyond triclinic crystals: out-of-equilibrium studies of Cp*ErCOT single-molecule magnet. <i>Chemistry - A European Journal</i> , 2013 , 19, 13726-31	4.8	62
50	A hydride-ligated dysprosium single-molecule magnet. <i>Chemical Communications</i> , 2013 , 49, 901-3	5.8	70
49	Relaxations in heterolanthanide dinuclear single-molecule magnets. <i>Chemical Communications</i> , 2013 , 49, 158-60	5.8	59
48	Magnetic anisotropy of CoIIWV ferromagnet: single crystal and ab initio study. <i>CrystEngComm</i> , 2013 , 15, 2378-2385	3.3	12
47	An organometallic building block approach to produce a multidecker 4f single-molecule magnet. <i>Journal of the American Chemical Society</i> , 2013 , 135, 3502-10	16.4	177
46	Synthesis and characterization of a two-coordinate manganese complex and its reaction with molecular hydrogen at room temperature. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 11817-21	16.4	73
45	By design: a macrocyclic 3d-4f single-molecule magnet with quantifiable zero-field slow relaxation of magnetization. <i>Inorganic Chemistry</i> , 2013 , 52, 3236-40	5.1	66
44	Interplay of strongly anisotropic metal ions in magnetic blocking of complexes. <i>Inorganic Chemistry</i> , 2013 , 52, 6328-37	5.1	203
43	Synthesis and Characterization of a Two-Coordinate Manganese Complex and its Reaction with Molecular Hydrogen at Room Temperature. <i>Angewandte Chemie</i> , 2013 , 125, 12033-12037	3.6	26
42	Net toroidal magnetic moment in the ground state of a {Dy6}-triethanolamine ring. <i>Journal of the American Chemical Society</i> , 2012 , 134, 18554-7	16.4	138
41	Coupling Dy3 triangles to maximize the toroidal moment. <i>Angewandte Chemie - International Edition</i> , 2012 , 51, 12767-71	16.4	191
40	Heterometallic tetranuclear [Ln(III)2Co(III)2] complexes including suppression of quantum tunneling of magnetization in the [Dy(III)2Co(III)2] single molecule magnet. <i>Inorganic Chemistry</i> , 2012 , 51, 11873-81	5.1	143
39	Coupling Dy3 Triangles to Maximize the Toroidal Moment. <i>Angewandte Chemie</i> , 2012 , 124, 12939-12943	3.6	33
38	Ab initio calculation of anisotropic magnetic properties of complexes. I. Unique definition of pseudospin Hamiltonians and their derivation. <i>Journal of Chemical Physics</i> , 2012 , 137, 064112	3.9	456
37	Heterometallic CuII/DyIII 1D chiral polymers: chirogenesis and exchange coupling of toroidal moments in trinuclear Dy3 single molecule magnets. <i>Chemical Science</i> , 2012 , 3, 1169	9.4	133
36	The first {Dy4} single-molecule magnet with a toroidal magnetic moment in the ground state. <i>Inorganic Chemistry</i> , 2012 , 51, 1233-5	5.1	177
35	Synthesis and magnetic properties of a new family of macrocyclic M(II)3Ln(III) complexes: insights into the effect of subtle chemical modification on single-molecule magnet behavior. <i>Inorganic Chemistry</i> , 2012 , 51, 10603-12	5.1	49
34	A single-molecule magnet assembly exhibiting a dielectric transition at 470 K. <i>Chemical Science</i> , 2012 , 3, 3366	9.4	150

33	Ytterbium can relax slowly too: a field-induced Yb ₂ single-molecule magnet. <i>Dalton Transactions</i> , 2012 , 41, 12349-52	4.3	68
32	A six-coordinate ytterbium complex exhibiting easy-plane anisotropy and field-induced single-ion magnet behavior. <i>Inorganic Chemistry</i> , 2012 , 51, 8538-44	5.1	204
31	Supramolecular architectures for controlling slow magnetic relaxation in field-induced single-molecule magnets. <i>Chemical Science</i> , 2012 , 3, 2158	9.4	140
30	Coexistence of Distinct Single-Ion and Exchange-Based Mechanisms for Blocking of Magnetization in a Co(II)Dy(III) ₂ Single-Molecule Magnet. <i>Angewandte Chemie</i> , 2012 , 124, 7668-7672	3.6	55
29	A High Anisotropy Barrier in a Sulfur-Bridged Organodysprosium Single-Molecule Magnet. <i>Angewandte Chemie</i> , 2012 , 124, 7082-7086	3.6	40
28	Coexistence of distinct single-ion and exchange-based mechanisms for blocking of magnetization in a Co(II) ₂ Dy(III) ₂ single-molecule magnet. <i>Angewandte Chemie - International Edition</i> , 2012 , 51, 7550-4	16.4	248
27	A high anisotropy barrier in a sulfur-bridged organodysprosium single-molecule magnet. <i>Angewandte Chemie - International Edition</i> , 2012 , 51, 6976-80	16.4	235
26	Hysteresis in the ground and excited spin state up to 10 T of a [Mn(III) ₆ Mn(III)] ³⁺ triplesalen single-molecule magnet. <i>Chemical Science</i> , 2012 , 3, 2868	9.4	35
25	From a Dy(III) single molecule magnet (SMM) to a ferromagnetic [Mn(II)Dy(III)Mn(II)] trinuclear complex. <i>Inorganic Chemistry</i> , 2012 , 51, 9589-97	5.1	105
24	Negative g factors, berry phases, and magnetic properties of complexes. <i>Physical Review Letters</i> , 2012 , 109, 246403	7.4	18
23	Single-molecule magnet behavior for an antiferromagnetically superexchange-coupled dinuclear dysprosium(III) complex. <i>Journal of the American Chemical Society</i> , 2011 , 133, 5319-28	16.4	485
22	Strong axiality and Ising exchange interaction suppress zero-field tunneling of magnetization of an asymmetric Dy ₂ single-molecule magnet. <i>Journal of the American Chemical Society</i> , 2011 , 133, 11948-51	16.4	604
21	Magnetic anisotropy in the excited states of low symmetry lanthanide complexes. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 20086-90	3.6	285
20	Symmetry related [Dy(III) ₆ Mn(III) ₁₂] cores with different magnetic anisotropies. <i>Chemical Science</i> , 2011 , 2, 1268	9.4	103
19	Synthesis, structure, magnetism and theoretical study of a series of complexes with a decanuclear core [Ln(III) ₂ Cu(II) ₈] (Ln = Y, Gd, Tb, Dy). <i>New Journal of Chemistry</i> , 2011 , 35, 1270	3.6	23
18	A Rare \bar{B} -O Centred Dy ₄ Tetrahedron with Coordination-Induced Local Chirality and Single-Molecule Magnet Behaviour. <i>European Journal of Inorganic Chemistry</i> , 2011 , 2011, 1535-1539	2.3	61
17	A Spectroscopic Investigation of Magnetic Exchange Between Highly Anisotropic Spin Centers. <i>Angewandte Chemie</i> , 2011 , 123, 4093-4097	3.6	1
16	A spectroscopic investigation of magnetic exchange between highly anisotropic spin centers. <i>Angewandte Chemie - International Edition</i> , 2011 , 50, 4007-11	16.4	31

15	Pure trinuclear 4f single-molecule magnets: synthesis, structures, magnetism and ab initio investigation. <i>Chemistry - A European Journal</i> , 2011 , 17, 2458-66	4.8	91
14	Structure, magnetism and theory of a family of nonanuclear Cu(II)5Ln(III)4-triethanolamine clusters displaying single-molecule magnet behaviour. <i>Chemistry - A European Journal</i> , 2011 , 17, 9209-18	4.8	105
13	A non-sandwiched macrocyclic monolanthanide single-molecule magnet: the key role of axiality. <i>Chemistry - A European Journal</i> , 2011 , 17, 4362-5	4.8	215
12	Back Cover: A Non-sandwiched Macrocyclic Monolanthanide Single-Molecule Magnet: The Key Role of Axiality (Chem. Eur. J. 16/2011). <i>Chemistry - A European Journal</i> , 2011 , 17, 4660-4660	4.8	
11	Ein achtkerniger [Cr(III)4Dy(III)4]-3d-4f-Einzelmolekülmagnet. <i>Angewandte Chemie</i> , 2010 , 122, 7746-7750	3.6	23
10	An octanuclear [Cr(III)4Dy(III)4] 3d-4f single-molecule magnet. <i>Angewandte Chemie - International Edition</i> , 2010 , 49, 7583-7	16.4	231
9	First heterotrimetallic {3 d-4 d-4 f} single chain magnet, constructed from anisotropic high-spin heterometallic nodes and paramagnetic spacers. <i>Chemistry - A European Journal</i> , 2009 , 15, 11808-14	4.8	194
8	A Polynuclear Lanthanide Single-Molecule Magnet with a Record Anisotropic Barrier. <i>Angewandte Chemie</i> , 2009 , 121, 9653-9656	3.6	76
7	A polynuclear lanthanide single-molecule magnet with a record anisotropic barrier. <i>Angewandte Chemie - International Edition</i> , 2009 , 48, 9489-92	16.4	535
6	Ab initio investigation of the non-collinear magnetic structure and the lowest magnetic excitations in dysprosium triangles. <i>New Journal of Chemistry</i> , 2009 , 33, 1224	3.6	269
5	Structure, magnetism, and theoretical study of a mixed-valence Co(II)3Co(III)4 heptanuclear wheel: lack of SMM behavior despite negative magnetic anisotropy. <i>Journal of the American Chemical Society</i> , 2008 , 130, 12445-55	16.4	363
4	The origin of nonmagnetic Kramers doublets in the ground state of dysprosium triangles: evidence for a toroidal magnetic moment. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 4126-9	16.4	514
3	The Origin of Nonmagnetic Kramers Doublets in the Ground State of Dysprosium Triangles: Evidence for a Toroidal Magnetic Moment. <i>Angewandte Chemie</i> , 2008 , 120, 4194-4197	3.6	109
2	A dinuclear cobalt(II) complex of calix[8]arenes exhibiting strong magnetic anisotropy. <i>Dalton Transactions</i> , 2007 , 4582-8	4.3	50
1	Toroidal magnetic moments in Tb4 squares. <i>Inorganic Chemistry Frontiers</i> ,	6.8	1