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List of Publications by Year
in descending order

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61 papers	3,145 citations	212478 28 h-index	175968 55 g-index
63 all docs	63 docs citations	63 times ranked	3773 citing authors

#	Article	IF	Citations
1	Azoâ€“hydrazone tautomerism in organometallic complexes triggered by a -Re(CO)3(L) core: A spectroscopic and theoretical study. Dyes and Pigments, 2022, 197, 109953.	2.0	2
2	Lanthanide SMMs Based on Belt Macrocycles: Recent Advances and General Trends. Chemistry - A European Journal, 2022, 28, .	1.7	11
3	Structure and excited-state dynamics of dimeric copper(i) photosensitizers investigated by time-resolved X-ray and optical transient absorption spectroscopy. Physical Chemistry Chemical Physics, 2021, 23, 3656-3667.	1.3	4
4	Nuclearity Control for Efficient Thermally Activated Delayed Fluorescence in a Cu^I Complex and its Halogen-Bridged Dimer. Chemistry of Materials, 2021, 33, 6383-6393.	3.2	12
5	Roomâ€Temperature Spinâ€Dependent Transport in Metalloporphyrinâ€Based Supramolecular Wires. Angewandte Chemie, 2021, 133, 26162-26169.	1.6	5
6	Roomâ€Temperature Spinâ€Dependent Transport in Metalloporphyrinâ€Based Supramolecular Wires. Angewandte Chemie - International Edition, 2021, 60, 25958-25965.	7.2	9
7	Single-Molecule Transport of Fullerene-Based Curcuminoids. Journal of Physical Chemistry C, 2020, 124, 2698-2704.	1.5	6
8	Reactivity of Cu^IN₄ Flattened Complexes: Interplay between Coordination Geometry and Ligand Flexibility. Inorganic Chemistry, 2020, 59, 15061-15073.	1.9	8
9	Control of magnetic anisotropy by macrocyclic ligand distortion in a family of Dy^{III}and Er^{III}single molecule magnets. Dalton Transactions, 2020, 49, 17709-17718.	1.6	14
10	Tuning Singleâ€Molecule Conductance in Metalloporphyrinâ€Based Wires via Supramolecular Interactions. Angewandte Chemie - International Edition, 2020, 59, 19193-19201.	7.2	19
11	High performance single-molecule magnets, Orbach or Raman relaxation suppression?. Inorganic Chemistry Frontiers, 2020, 7, 2478-2486.	3.0	76
12	Spin dynamics in single-molecule magnets and molecular qubits. Dalton Transactions, 2020, 49, 9916-9928.	1.6	82
13	Effect of Second-Sphere Interactions on the Magnetic Anisotropy of Lanthanide Single-Molecule Magnets: Electrostatic Interactions and Supramolecular Contacts. Journal of Physical Chemistry C, 2020, 124, 5308-5320.	1.5	14
14	[UF 6] 2â^' : A Molecular Hexafluorido Actinide(IV) Complex with Compensating Spin and Orbital Magnetic Moments. Angewandte Chemie - International Edition, 2019, 58, 15650-15654.	7.2	8
15	[UF 6] 2â^' : A Molecular Hexafluorido Actinide(IV) Complex with Compensating Spin and Orbital Magnetic Moments. Angewandte Chemie, 2019, 131, 15797-15801.	1.6	0
16	RÃ¼cktitelbild: [UF₆]^{2â^'}: A Molecular Hexafluorido Actinide(IV) Complex with Compensating Spin and Orbital Magnetic Moments (Angew. Chem. 44/2019). Angewandte Chemie, 2019, 131, 16084-16084.	1.6	0
17	Relaxation time enhancement by magnetic dilution in single-molecule magnets: An ab initio study. Journal of Magnetism and Magnetic Materials, 2019, 489, 165456.	1.0	18
18	Influence of the channel size of isostructural 3dâ€“4f MOFs on the catalytic aerobic oxidation of cycloalkenes. New Journal of Chemistry, 2019, 43, 11057-11064.	1.4	13

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19	Influence of the substituent on the phosphine ligand in novel rhenium(<scp>i</scp>) aldehydes. Synthesis, computational studies and first insights into the antiproliferative activity. Dalton Transactions, 2018, 47, 13861-13869.	1.6	14
20	Ab Initio Prediction of Tunneling Relaxation Times and Effective Demagnetization Barriers in Kramers Lanthanide Single-Molecule Magnets. Journal of Physical Chemistry Letters, 2018, 9, 5327-5333.	2.1	69
21	Designing a Dy₂ Single-Molecule Magnet with Two Well-Differentiated Relaxation Processes by Using a Nonsymmetric Bis-bidentate Bipyrimidine-N-Oxide Ligand: A Comparison with Mononuclear Counterparts. Inorganic Chemistry, 2018, 57, 6362-6375.	1.9	54
22	Effect of Heteroatoms on Field-Induced Slow Magnetic Relaxation of Mononuclear Fe^{III} (S = 5/2) Ions within Polyoxometalates. Inorganic Chemistry, 2018, 57, 6957-6964.	1.9	16
23	Steric and Electronic Factors Affecting the Conformation of Bimetallic Cu^I Complexes: Effect of the Aliphatic Spacer of Tetracoordinating Schiffâ€Base Ligands. Chemistry - A European Journal, 2018, 24, 13839-13849.	1.7	18
24	Effect of Low Spin Excited States for Magnetic Anisotropy of Transition Metal Mononuclear Single Molecule Magnets. Inorganics, 2018, 6, 24.	1.2	2
25	Solid state photoluminescence studies of [EuLnH2(NO3)3](H2O)x macrocyclic complexes with Schiff base ligands. Journal of Luminescence, 2018, 203, 7-15.	1.5	6
26	Metal-Controlled Magnetoresistance at Room Temperature in Single-Molecule Devices. Journal of the American Chemical Society, 2017, 139, 5768-5778.	6.6	41
27	Models to predict the magnetic properties of single- and multiple-bridged phosphate Cu^{II} systems: a theoretical DFT insight. Inorganic Chemistry Frontiers, 2017, 4, 509-520.	3.0	6
28	Influence of the lanthanide(iii) ion in {[Cu3Ln2(oda)6(H2O)6]Â·nH2O}n (LnIII: La, Gd, Yb) catalysts on the heterogeneous oxidation of olefins. Catalysis Science and Technology, 2017, 7, 231-242.	2.1	13
29	Charge Transport through a Single Molecule of trans-1-bis-Diazofluorene [60]fullerene. Chemistry of Materials, 2017, 29, 7305-7312.	3.2	3
30	Effect of the substituent of the cation of N-octylpyridinium hexafluorophosphate in the electrical and electrochemical response of carbon paste electrodes modified with these ionic liquids. Electrochimica Acta, 2017, 258, 959-969.	2.6	7
31	Periodic Trends in Lanthanide Compounds through the Eyes of Multireference ab Initio Theory. Inorganic Chemistry, 2016, 55, 4457-4469.	1.9	98
32	Frontispiece: Lanthanide Tetrazolate Complexes Combining Single-Molecule Magnet and Luminescence Properties: The Effect of the Replacement of Tetrazolate N3 by Î²-Diketonate Ligands on the Anisotropy Energy Barrier. Chemistry - A European Journal, 2016, 22, .	1.7	0
33	Exchange Interactions on the Highest-Spin Reported Molecule: the Mixed-Valence Fe42 Complex. Scientific Reports, 2016, 6, 23847.	1.6	15
34	DFT approaches to transport calculations in magnetic single-molecule devices. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	8
35	Lanthanide Tetrazolate Complexes Combining Singleâ€Molecule Magnet and Luminescence Properties: The Effect of the Replacement of Tetrazolate N₃ by Î²â€Diketonate Ligands on the Anisotropy Energy Barrier. Chemistry - A European Journal, 2016, 22, 14548-14559.	1.7	48
36	A low spin manganese(<scp>iv</scp>) nitride single molecule magnet. Chemical Science, 2016, 7, 6132-6140.	3.7	112

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37	Single-Molecule Magnet Properties of Transition-Metal Ions Encapsulated in Lacunary Polyoxometalates: A Theoretical Study. Inorganic Chemistry, 2016, 55, 6405-6413.	1.9	23
38	Improved Segmented All-Electron Relativistically Contracted Basis Sets for the Lanthanides. Journal of Chemical Theory and Computation, 2016, 12, 1148-1156.	2.3	112
39	Large Conductance Switching in a Single-Molecule Device through Room Temperature Spin-Dependent Transport. Nano Letters, 2016, 16, 218-226.	4.5	148
40	Large magnetic anisotropy in mononuclear metal complexes. Coordination Chemistry Reviews, 2015, 289-290, 379-392.	9.5	339
41	Increasing the effective energy barrier promoted by the change of a counteranion in a Znâ€“Dyâ€“Zn SMM: slow relaxation via the second excited state. Chemical Communications, 2015, 51, 12353-12356.	2.2	59
42	First evidence of light-induced spin transition in molybdenum(<scp>iv</scp>). Chemical Communications, 2015, 51, 8229-8232.	2.2	60
43	Neodymium 1D systems: targeting new sources for field-induced slow magnetization relaxation. Dalton Transactions, 2015, 44, 15774-15778.	1.6	33
44	First principles approach to the electronic structure, magnetic anisotropy and spin relaxation in mononuclear 3d-transition metal single molecule magnets. Coordination Chemistry Reviews, 2015, 289-290, 177-214.	9.5	267
45	Two C₃â€Symmetric Dy₃^{III} Complexes with Triple Diâ€Î¼â€methoxoâ€Î¼â€phenoxo Bridges, Magnetic Ground State, and Singleâ€Molecule Magnetic Behavior. Chemistry - A European Journal, 2014, 20, 8410-8420.	1.7	40
46	Spin-Crossover Behavior in Two New Supramolecular Isomers. Inorganic Chemistry, 2014, 53, 201-208.	1.9	23
47	Guest Modulation of Spinâ€Crossover Transition Temperature in a Porous Iron(II) Metalâ€“Organic Framework: Experimental and Periodic DFT Studies. Chemistry - A European Journal, 2014, 20, 12864-12873.	1.7	55
48	Rational Electrostatic Design of Easyâ€Axis Magnetic Anisotropy in a Zn^{II}â€“Dy^{III}â€“Zn^{II} Singleâ€Molecule Magnet with a High Energy Barrier. Chemistry - A European Journal, 2014, 20, 14262-14269.	1.7	95
49	Effect of Metal Complexation on the Conductance of Single-Molecular Wires Measured at Room Temperature. Journal of the American Chemical Society, 2014, 136, 8314-8322.	6.6	45
50	Two 3dâ€“4f nanomagnets formed via a two-step in situ reaction of picolinaldehyde. Chemical Communications, 2013, 49, 6549.	2.2	69
51	Shedding Light on the Single-Molecule Magnet Behavior of Mononuclear Dy^{III} Complexes. Inorganic Chemistry, 2013, 52, 13770-13778.	1.9	176
52	Unprecedented ferromagnetic dipolar interaction in a dinuclear holmium(iii) complex: a combined experimental and theoretical study. Chemical Communications, 2013, 49, 9341.	2.2	32
53	Spins on a curved surface: an FeIII14 ferracalixarene. Dalton Transactions, 2013, 42, 9606.	1.6	6
54	Cu^{II}ï£¿Gd^{III} Cryogenic Magnetic Refrigerants and Cu₈Dy₉ Singleâ€Molecule Magnet Generated by In Situ Reactions of Picolinaldehyde and Acetylpyridine: Experimental and Theoretical Study. Chemistry - A European Journal, 2013, 19, 17567-17577.	1.7	88

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55	Reversible Chemisorption of Sulfur Dioxide in a Spin Crossover Porous Coordination Polymer. Inorganic Chemistry, 2013, 52, 12777-12783.	1.9	72
56	Coherent Transport through Spin-Crossover Single Molecules. Journal of the American Chemical Society, 2012, 134, 777-779.	6.6	140
57	Enhanced bistability by guest inclusion in Fe(ii) spin crossover porous coordination polymers. Chemical Communications, 2012, 48, 4686.	2.2	107
58	Hexanuclear Copper(II) Cages Built on a Central {Î¼₃â€“OÂ·Â·Â·HÂ·Â·Â·Î¼₃â€“O} Moiety, 1,3-Bis(dimethylamino)-2-propanolato and Capping R-phosphonates: Crystal Structures, Magnetic Behavior, and DFT Studies. Inorganic Chemistry, 2012, 51, 6842-6850.	1.9	20
59	Theoretical Study of Exchange Coupling in 3d-Gd Complexes: Large Magnetocaloric Effect Systems. Journal of the American Chemical Society, 2012, 134, 10532-10542.	6.6	154
60	The Dilemma of Cr^{III}Ni^{II} Exchange Interactions: Ferromagnetism versus Antiferromagnetism. Chemistry - A European Journal, 2011, 17, 8841-8849.	1.7	3
61	Structural and electronic effects on the exchange interactions in dinuclear bis(phenoxo)-bridged copper(II) complexes. Coordination Chemistry Reviews, 2010, 254, 2086-2095.	9.5	148