Coen de Graaf

List of Publications by Year
in descending order

174 papers	6,235 citations	70961 41 h-index	88477 70 g-index
182 all docs	182 docs citations	182 times ranked	5394 citing authors

#	Article	IF	Citations
1	Managing the Computational Chemistry Big Data Problem: The ioChem-BD Platform. Journal of Chemical Information and Modeling, 2015, 55, 95-103.	2.5	403
2	Magnetic Interactions in Molecules and Highly Correlated Materials: Physical Content, Analytical Derivation, and Rigorous Extraction of Magnetic Hamiltonians. Chemical Reviews, 2014, 114, 429-492.	23.0	342
3	Universal Theoretical Approach to Extract Anisotropic Spin Hamiltonians. Journal of Chemical Theory and Computation, 2009, 5, 2977-2984.	2.3	270
4	Magnetic coupling in biradicals, binuclear complexes and wide-gap insulators: a survey of ab initio wave function and density functional theory approaches. Theoretical Chemistry Accounts, 2000, 104, 265-272.	0.5	268
5	Polyoxometalates with Internal Cavities:â€‰ Redox Activity, Basicity, and Cation Encapsulation in [Xⁿ⁺P₅W₃₀O₁₁₀]⁽¹⁵⁻ⁿ/s Preyssler Complexes, with X = Na⁺, Ca²⁺, Y³⁺, La³⁺, Ce³⁺, and Th⁴⁺. Journal of the American Chemical Society, 2007, 129, 12244-12253.	6.6	152
6	Artificial chemical and magnetic structure at the domain walls of an epitaxial oxide. Nature, 2014, 515, 379-383.	13.7	146
7	Origin of the Magnetic Anisotropy in Heptacoordinate Ni^{II} and Co^{II} Complexes. Chemistry - A European Journal, 2013, 19, 950-956.	1.7	145
8	Ultrafast Deactivation Mechanism of the Excited Singlet in the Lightâ€‰induced Spin Crossover of [Fe(2,2â€²â€‰bipyridine)₃]²⁺. Chemistry - A European Journal, 2013, 19, 17541-17551.	1.7	145
9	Multiconfigurational Perturbation Theory:Â An Efficient Tool to Predict Magnetic Coupling Parameters in Biradicals, Molecular Complexes, and Ionic Insulators. Journal of Physical Chemistry A, 2001, 105, 11371-11378.	1.1	129
10	Ab Initio Study of the Exchange Coupling in Oxalato-Bridged Cu(II) Dinuclear Complexes. Journal of Physical Chemistry A, 2000, 104, 9983-9989.	1.1	103
11	U₂@I_h(7)-C₈₀: Crystallographic Characterization of a Long-Sought Dimetallic Actinide Endohedral Fullerene. Journal of the American Chemical Society, 2018, 140, 3907-3915.	6.6	96
12	Theoretical Determination of the Zero-Field Splitting in Copper Acetate Monohydrate. Inorganic Chemistry, 2011, 50, 6229-6236.	1.9	91
13	Study of the Lightâ€‰induced Spin Crossover Process of the [Fe^{II}(bpy)₃]²⁺ Complex. Chemistry - A European Journal, 2010, 16, 4550-4556.	1.7	86
14	Theoretical Investigation of the Electronic Structure of Fe(II) Complexes at Spin-State Transitions. Journal of Chemical Theory and Computation, 2013, 9, 509-519.	2.3	85
15	On the applicability of multireference secondâ€‰order perturbation theory to study weak magnetic coupling in molecular complexes. Journal of Computational Chemistry, 2008, 29, 994-1003.	1.5	84
16	Electronic Structure and Redox Properties of Metal Nitride Endohedral Fullerenes M₃N@C_{2n} (M=Sc, Y, La, and Gd; 2n=80, 84, 88, 92, 96). Chemistry - A European Journal, 2009, 15, 10997-11009.	1.7	84
17	Role of the Coordination of the Azido Bridge in the Magnetic Coupling of Copper(II) Binuclear Complexes. Chemistry - A European Journal, 2003, 9, 2307-2315.	1.7	80
18	Light-Induced Excited-State Spin Trapping in Tetrazole-Based Spin Crossover Systems. Journal of the American Chemical Society, 2008, 130, 13961-13968.	6.6	79

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19	Rigorous Extraction of the Anisotropic Multispin Hamiltonian in Bimetallic Complexes from the Exact Electronic Hamiltonian. Journal of Chemical Theory and Computation, 2010, 6, 55-65.	2.3	76
20	Energetics of [Fe(NCH)₆]²⁺ via CASPT2 calculations: A spinâ€crossover perspective. Journal of Computational Chemistry, 2009, 30, 2327-2333.	1.5	61
21	Ab initiostudy of the magnetic interactions in the spin-ladder compoundSrCu2O3. Physical Review B, 1999, 60, 3457-3464.	1.1	60
22	Four-spin cyclic exchange in spin ladder cuprates. Physical Review B, 2003, 67, .	1.1	59
23	Ferromagnetism and increased ionicity in epitaxially grownTbMnO3films. Physical Review B, 2009, 79, .	1.1	58
24	Photoreduction Mechanism of CO₂ to CO Catalyzed by a Rhenium(I)â€“Polyoxometalate Hybrid Compound. ACS Catalysis, 2016, 6, 6422-6428.	5.5	58
25	Magnetic structure ofLi2CuO2:â€ƒFromab initiocalculations to macroscopic simulations. Physical Review B, 2002, 66, .	1.1	57
26	Computational approach to the study of thermal spin crossover phenomena. Journal of Chemical Physics, 2014, 140, 184318.	1.2	57
27	Electronic structure and magnetic interactions of the spin-chain compoundsCa2CuO3andSr2CuO3. Physical Review B, 2000, 63, .	1.1	56
28	Magnetostructural relations from a combined ab initio and ligand field analysis for the nonintuitive zero-field splitting in Mn(III) complexes. Journal of Chemical Physics, 2010, 133, 084307.	1.2	54
29	Antisymmetric Magnetic Interactions in Oxo-Bridged Copper(II) Bimetallic Systems. Journal of Chemical Theory and Computation, 2010, 6, 3092-3101.	2.3	51
30	Absence of collective effects in Heisenberg systems with localized magnetic moments. Physical Review B, 1997, 56, 5069-5072.	1.1	50
31	Addressing Multiple Resistive States of Polyoxovanadates: Conductivity as a Function of Individual Molecular Redox States. Journal of the American Chemical Society, 2018, 140, 16635-16640.	6.6	49
32	Further Theoretical Evidence for the Exceptionally Strong Ferromagnetic Coupling in Oxo-Bridged Cu(II) Dinuclear Complexes. Journal of Physical Chemistry A, 2002, 106, 4938-4941.	1.1	48
33	Microscopic origin of isotropic non-Heisenberg behavior in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>S</mml:mi><mml:mo>=</mml:mo><mml:mn>1</mml:mn></mml:mrow></mml:math>magnetic systems. Physical Review B, 2007, 76, .	1.1	48
34	On the magnetic coupling in NiO. Journal of Chemical Physics, 1997, 106, 3287-3291.	1.2	46
35	Spin crossover in Fe(II) complexes: An ab initio study of ligand Ïâ€donation. International Journal of Quantum Chemistry, 2010, 110, 331-337.	1.0	46
36	On the role of the metalâ€toâ€ligand charge transfer states in the lightâ€induced spin crossover in Fe^{II} (bpy)₃. International Journal of Quantum Chemistry, 2011, 111, 3385-3393.	1.0	46

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37	Theoretical determination of spin Hamiltonians with isotropic and anisotropic magnetic interactions in transition metal and lanthanide complexes. Physical Chemistry Chemical Physics, 2013, 15, 18784.	1.3	45
38	Magneto-structural correlations in binuclear copper(ii) compounds bridged by a ferrocenecarboxylato(â€“1) and an hydroxo- or methoxo-ligands. Dalton Transactions, 2005, , 2322.	1.6	44
39	Isotropic non-Heisenberg terms in the magnetic coupling of transition metal complexes. Journal of Chemical Physics, 2008, 129, 104102.	1.2	43
40	Comparison of the superexchange interaction in NiO and in a NiO[100] surface. Chemical Physics Letters, 1997, 271, 372-376.	1.2	42
41	Ab initioabsorption spectrum of NiO combining molecular dynamics with the embedded cluster approach in a discrete reaction field. Physical Review B, 2012, 85, .	1.1	42
42	Midinfrared spectrum of undoped cuprates:â€ƒd-dtransitions studied byab initiomethods. Physical Review B, 2000, 62, 702-709.	1.1	41
43	Density Functional Theory and ab Initio Study of Electronic and Electrochemistry Properties of the Tetranuclear Sandwich Complex [FeIII4(H2O)2(PW9O34)2]6-. Inorganic Chemistry, 2007, 46, 4022-4027.	1.9	40
44	A comparative synthetic, magnetic and theoretical study of functional M4Cl4 cubane-type Co(ii) and Ni(ii) complexes. Dalton Transactions, 2014, 43, 7847.	1.6	40
45	Putting error bars on theAb Initiotheoretical estimates of the magnetic coupling constants: The parent compounds of superconducting cuprates as a case study. Journal of Computational Chemistry, 2004, 25, 1234-1241.	1.5	39
46	Magnetic anisotropy in binuclear complexes in the weak-exchange limit: From the multispin to the giant-spin Hamiltonian. Physical Review B, 2010, 81, .	1.1	39
47	Role of charge transfer configurations in LaMnO3, CaMnO3, and CaFeO3. Journal of Chemical Physics, 2007, 126, 134709.	1.2	38
48	Detailed ab-initio analysis of the magnetic coupling in CuF2. Chemical Physics Letters, 2000, 319, 625-630.	1.2	37
49	Quantum chemical study of the nature of the ground state and the pressure-induced spin transition inCaFeO3. Physical Review B, 2007, 75, .	1.1	36
50	Interplay between Local Anisotropies in Binuclear Complexes. Inorganic Chemistry, 2014, 53, 4508-4516.	1.9	36
51	Assessing the zero-field splitting in magnetic molecules by wave function-based methods. International Journal of Quantum Chemistry, 2006, 106, 2470-2478.	1.0	35
52	Characterization of a strong covalent Th3+â€“Th3+ bond inside an Ih(7)-C80 fullerene cage. Nature Communications, 2021, 12, 2372.	5.8	34
53	Magnetic Interactions in Molecules and Solids. Theoretical Chemistry and Computational Modelling, 2016, , .	0.2	32
54	Optical properties of peroxy radicals in silica: Multiconfigurational perturbation theory calculations. Journal of Chemical Physics, 2001, 114, 6259-6264.	1.2	31

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55	Toward a variational treatment of the magnetic coupling between centers with elevated spin moments. Chemical Physics, 2005, 309, 259-269.	0.9	31
56	On the Heisenberg behaviour of magnetic coupling in the manganese dimer. Chemical Physics Letters, 2008, 458, 290-294.	1.2	31
57	Analysis of the magnetic coupling in nitroxide organic biradicals. Theoretical Chemistry Accounts, 2011, 128, 505-519.	0.5	31
58	Metal-to-metal charge-transfer transitions: reliable excitation energies from ab initio calculations. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	31
59	Ionization and excitation energies in CuCl and NiO within different embedding schemes. Computational and Theoretical Chemistry, 1998, 458, 53-60.	1.5	30
60	On the mechanism of the photoinduced magnetism in copper octacyanomolybdates. Chemical Communications, 2010, 46, 5737.	2.2	30
61	Dicobalt-Î¼-oxo Polyoxometalate Compound, [(Î±₂-P₂W₁₇O₆₁Co)₂O]^{14â€“}: A Potent Species for Water Oxidation, Câ€“H Bond Activation, and Oxygen Transfer. Inorganic Chemistry, 2014, 53, 1779-1787.	1.9	30
62	Photoinduced Moâ^'CN Bond Breakage in Octacyanomolybdate Leading to Spin Triplet Trapping. Angewandte Chemie - International Edition, 2020, 59, 3117-3121.	7.2	30
63	Electronic structure ofCaCu2O3: Spin ladder versus one-dimensional spin chain. Physical Review B, 2005, 71, .	1.1	29
64	Insights on the photomagnetism in copper octacyanomolybdates. Dalton Transactions, 2011, 40, 7295.	1.6	29
65	The Absorption Spectrum of Cytosine Tautomers: Beyond the Static Approach. Journal of Chemical Theory and Computation, 2012, 8, 235-244.	2.3	29
66	TD-DFT study of the light-induced spin crossover of Fe(<scp>iii</scp>) complexes. Physical Chemistry Chemical Physics, 2016, 18, 1233-1244.	1.3	29
67	Theoretical evidence for the direct ³MLCT-HS deactivation in the light-induced spin crossover of Fe(<scp>ii</scp>)â€“polypyridyl complexes. Physical Chemistry Chemical Physics, 2018, 20, 2351-2355.	1.3	29
68	Theoretical Characterization of the Ground and Optically Excited States ofÎ±â€²â^'NaV2O5. Physical Review Letters, 2002, 89, 076407.	2.9	27
69	On the role of relaxed charge-transfer excitations: Ni 3s hole states in NiO. Chemical Physics Letters, 1997, 272, 341-346.	1.2	26
70	Magnetic interactions in calcium and sodium ladder vanadates. Journal of Chemical Physics, 2004, 120, 961-967.	1.2	26
71	Highly Reduced Polyoxometalates:Â Ab Initio and DFT Study of [PMo8V4O40(VO)4]5-. Journal of Chemical Theory and Computation, 2005, 1, 856-861.	2.3	26
72	First-principles study of magnetic interactions in cupric oxide. Physical Review B, 2012, 85, .	1.1	26

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73	Switchable Rashba anisotropy in layered hybrid organicâ€“inorganic perovskite by hybrid improper ferroelectricity. Npj Computational Materials, 2020, 6, .	3.5	26
74	Theoretical study of local electronic transitions in the NiO(100) surface. Surface Science, 1999, 421, 106-115.	0.8	25
75	Quantum Chemical Characterization of Single Molecule Magnets Based on Uranium. Journal of Physical Chemistry A, 2017, 121, 1726-1733.	1.1	25
76	U₂N@I_h(7)-C₈₀: fullerene cage encapsulating an unsymmetrical U(<scp>iv</scp>)îNîU(<scp>v</scp>) cluster. Chemical Science, 2021, 12, 282-292.	3.7	25
77	The electronic structure of Ullman's biradicals: an orthogonal valence bond interpretation. Physical Chemistry Chemical Physics, 2011, 13, 14617.	1.3	24
78	Jahnâ€“Teller effect in Ag2+ doped KCl and NaCl: Is there any influence of the host lattice?. Chemical Physics Letters, 2006, 430, 51-55.	1.2	23
79	Magnetic interactions in LiCu2O2: Single-chain versus double-chain models. Physical Review B, 2012, 86, .	1.1	23
80	Theoretical Study of the Light-Induced Spin Crossover Mechanism in [Fe(mtz)₆]²⁺ and [Fe(phen)₃]²⁺. Journal of Physical Chemistry A, 2017, 121, 9720-9727.	1.1	23
81	Electronic structureÎ±â€²â^'NaV2O5:Wave-function-based embedded-cluster calculations. Physical Review B, 2003, 67, .	1.1	22
82	Computation of the energyV0of an excess electron in dense helium and argon. Journal of Chemical Physics, 1993, 98, 592-601.	1.2	21
83	Analysis of the Magnetic Coupling in M₃(dpa)₄Cl₂Systems (M = Ni,) Tj ETQq1 1 0.784314 rgBT	1.1	21
84	Insights from Adsorption and Electron Modification Studies of Polyoxometalates on Surfaces for Molecular Memory Applications. Accounts of Chemical Research, 2021, 54, 3377-3389.	7.6	21
85	The electronic structure of NiO for Ni 3s-hole states including full orbital relaxation and localization. Journal of Electron Spectroscopy and Related Phenomena, 1999, 98-99, 303-319.	0.8	20
86	Electric field effects on the ionic-neutral curve crossing of alkali halide molecules. Journal of Chemical Physics, 2000, 113, 9940-9947.	1.2	20
87	Improving the calculation of magnetic coupling constants in MRPT methods. Journal of Computational Chemistry, 2014, 35, 1665-1671.	1.5	20
88	GronOR: Massively parallel and GPU-accelerated non-orthogonal configuration interaction for large molecular systems. Journal of Chemical Physics, 2020, 152, 064111.	1.2	20
89	Reduced Common Molecular Orbital Basis for Nonorthogonal Configuration Interaction. Journal of Chemical Theory and Computation, 2020, 16, 2941-2951.	2.3	20
90	Effect of Secondâ€Order Spinâ€“Orbit Coupling on the Interaction between Spin States in Spinâ€Crossover Systems. Chemistry - A European Journal, 2018, 24, 5146-5152.	1.7	19

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91	Deactivation of Excited States in Transitionâ€Metal Complexes: Insight from Computational Chemistry. Chemistry - A European Journal, 2019, 25, 1152-1164.	1.7	19
92	Photoreduction Mechanism of CO₂ to CO Catalyzed by a Three-Component Hybrid Construct with a Bimetallic Rhenium Catalyst. ACS Catalysis, 2021, 11, 1495-1504.	5.5	19
93	Theoretical study of the crystal field excitations in CoO. Chemical Physics, 1998, 237, 59-65.	0.9	18
94	Neutral atoms in ionic lattices:â€ƒExcited states ofKCl:Ag0. Physical Review B, 2000, 62, 13366-13375.	1.1	18
95	Competition between double exchange and purely magnetic Heisenberg models in mixed valence systems: Application to half-doped manganites. Journal of Chemical Physics, 2006, 125, 194708.	1.2	18
96	Ab initiostudy of the CE magnetic phase in half-doped manganites: Purely magnetic versus double exchange description. Physical Review B, 2008, 77, .	1.1	18
97	Ab initio study of the singlet-triplet splitting in reduced polyoxometalates. Theoretical Chemistry Accounts, 2009, 123, 3-10.	0.5	18
98	Impact of short and long-range effects on the magnetic interactions in neutral organic radical-based materials. Physical Chemistry Chemical Physics, 2013, 15, 6982.	1.3	18
99	How Does the Redox State of Polyoxovanadates Influence the Collective Behavior in Solution? A Case Study with [I@V18O42]qâ^' (q = 3, 5, 7, 11, and 13). Inorganic Chemistry, 2019, 58, 3881-3894.	1.9	18
100	Core exciton energies of bulk MgO,Al2O3,andSiO2from explicitly correlatedab initiocluster model calculations. Physical Review B, 2000, 62, 10013-10021.	1.1	17
101	Ferrimagnetic coupling in oxamido-bridged Mn(II)Cu(II) compounds: a combined CASPT2 and DDCI study. Molecular Physics, 2003, 101, 2095-2102.	0.8	17
102	Ab initiostudy of the charge order and Zener polaron formation in half-doped manganites. Physical Review B, 2004, 70, .	1.1	17
103	CASSCF study of the relation between the Fe charge and the MÃ¶ssbauer isomer shift. Chemical Physics Letters, 2008, 454, 196-200.	1.2	17
104	Spin-crossover in phenylazopyridine-functionalized Niâ€“porphyrin: transâ€“cis isomerization triggered by Ï€â€“Ï€ interactions. Physical Chemistry Chemical Physics, 2015, 17, 217-225.	1.3	17
105	Role of the Imide Axial Ligand in the Spin and Oxidation State of Manganese Corrole and Corrolazine Complexes. Inorganic Chemistry, 2016, 55, 5274-5280.	1.9	17
106	A relationship between electronic structure effective parameters and Tc in monolayered cuprate superconductors. Chemical Physics Letters, 2001, 345, 183-188.	1.2	16
107	Ab initio study of the magnetic coupling in oxalato-bridged dinuclear Ni(II) complexes. Computational and Theoretical Chemistry, 2005, 727, 173-179.	1.5	16
108	Hopping matrix elements from first-principles studies of overlapping fragments: Double exchange parameters in manganites. International Journal of Quantum Chemistry, 2006, 106, 2444-2457.	1.0	16

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109	On the magnetic coupling in asymmetric bridged Cu(II) dinuclear complexes: The influence of substitutions on the carboxylato group. Inorganica Chimica Acta, 2011, 375, 166-172.	1.2	16
110	The effect of thermal motion on the electron localization in metal-to-ligand charge transfer excitations in [Fe(bpy)₃]²⁺. Dalton Transactions, 2014, 43, 17838-17846.	1.6	16
111	The magnetic fingerprint of dithiazolyl-based molecule magnets. Physical Chemistry Chemical Physics, 2018, 20, 20406-20416.	1.3	16
112	Explanation of the site-specific spin crossover in Fe(mtz)6(BF4)2. Dalton Transactions, 2013, 42, 14702.	1.6	15
113	Reconciling the valence state with magnetism in mixed-valent polyoxometalates: the case of a {VO₂F₂@V₂₂O₅₄} cluster. Physical Chemistry Chemical Physics, 2017, 19, 29767-29771.	1.3	15
114	Phenylazopyridine as Switch in Photochemical Reactions. A Detailed Computational Description of the Mechanism of Its Photoisomerization. Materials, 2017, 10, 1342.	1.3	15
115	Pre-exascale accelerated application development: The ORNL Summit experience. IBM Journal of Research and Development, 2020, 64, 11:1-11:21.	3.2	15
116	Molecular Transition Metal Oxide Electrocatalysts for the Reversible Carbon Dioxideâ€“Carbon Monoxide Transformation. Angewandte Chemie - International Edition, 2022, 61, .	7.2	15
117	Ab initiostudy of the Zener polaron spectrum of half-doped manganites: Comparison of several model Hamiltonians. Physical Review B, 2006, 74, .	1.1	14
118	Isotropic Non-Heisenberg Behavior in M₃(dpa)₄Cl₂ Extended Metal Atom Chains. Journal of Physical Chemistry A, 2010, 114, 12291-12298.	1.1	14
119	Electronic reorganization triggered by electron transfer: The intervalence charge transfer of a Fe³⁺/Fe²⁺ bimetallic complex. Journal of Computational Chemistry, 2015, 36, 861-869.	1.5	14
120	Is it possible to use Charge Transfer Bands to Measure Impurity-Ligand Distances? Experimental and Theoretical Results on Cu 2+ Doped (C 2 H 5 NH 3) 2 CdCl 4. High Pressure Research, 2002, 22, 475-478.	0.4	13
121	Ab initio and DFT study of the exchange coupling in the highly reduced polyoxoanion [PMo12O40(VO)2]5â^'. Chemical Physics Letters, 2006, 428, 88-92.	1.2	13
122	Ni 3s-hole states in NiO by non-orthogonal configuration interaction. Chemical Physics, 2006, 331, 178-185.	0.9	13
123	Neutral atoms in ionic lattices:â€ƒStability and ground-state properties ofKCl:Ag0. Physical Review B, 2000, 62, 13356-13365.	1.1	12
124	Magnetic coupling in oxalato-bridged hetero-bimetallic compounds: an ab initio study. Polyhedron, 2003, 22, 2409-2414.	1.0	12
125	Accuracy of Embedded Fragment Calculation for Evaluating Electron Interactions in Mixed Valence Magnetic Systems: Study of 2e-Reduced Lindqvist Polyoxometalates. Journal of Chemical Theory and Computation, 2015, 11, 550-559.	2.3	12
126	Biradical character in the ground state of [Mn@Si₁₂]⁺: a DFT and CASPT2 study. Physical Chemistry Chemical Physics, 2016, 18, 24006-24014.	1.3	12

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127	Influence of the crystal packing in singlet fission: one step beyond the gas phase approximation. Physical Chemistry Chemical Physics, 2021, 23, 14164-14177.	1.3	12
128	Ab initiotheory of magnetic interactions at surfaces. Journal of Physics Condensed Matter, 2004, 16, S2557-S2574.	0.7	11
129	On the role of solvent effects on the electronic transitions in Fe(II) and Ru(II) complexes. Chemical Physics, 2014, 428, 59-66.	0.9	11
130	Accurate Determination of the Electronic Structure Parameters of the Spin Ladder Compounds SrCu2O3, Sr2Cu3O5 and CaCu2O3. Theoretical Chemistry Accounts, 2006, 116, 535-548.	0.5	10
131	Ab initio study of the antiferromagnetic coupling in the wheel-shaped [Cu20Cl(OH)24(H2O)12(P8W48O184)]25â€“ anion. Physical Chemistry Chemical Physics, 2010, 12, 2716.	1.3	10
132	A multiconfigurational approach to the electronic structure of trichromium extended metal atom chains. Dalton Transactions, 2017, 46, 6202-6211.	1.6	10
133	Controlling the Lifetime of the Triplet MLCT State in Fe(II) Polypyridyl Complexes through Ligand Modification. Inorganics, 2020, 8, 16.	1.2	10
134	Ultrafast Intersystem Crossing in Xanthone from Wavepacket Dynamics. Journal of the American Chemical Society, 2021, 143, 21474-21477.	6.6	10
135	Optical spectroscopy of (C2H5NH3)2CdCl4:Cu2+under pressure: Study of Cu2+local structure from theoretical calculations. International Journal of Quantum Chemistry, 2002, 86, 239-244.	1.0	9
136	Unexpected role of Madelung potential in monoplanar high-Tc cuprate superconductors. Chemical Physics Letters, 2003, 379, 291-296.	1.2	9
137	Renormalization of quasiparticle hopping integrals by spin interactions in layered copper oxides. Physical Review B, 2007, 75, .	1.1	9
138	H₂Sâ€Mediated Thermal and Photochemical Methane Activation. ChemPhysChem, 2013, 14, 3960-3970.	1.0	9
139	Quantum Chemical Study of the Interligand Electron Transfer in Ru Polypyridyl Complexes. Journal of Physical Chemistry A, 2018, 122, 1114-1123.	1.1	9
140	Decoding the role of encapsulated ions in the electronic and magnetic properties of mixed-valence polyoxovanadate capsules {X@V₂₂O₅₄} (X = ClO₄^{â^’},) Tj ETQq0 0 0 rgBT /Overloc Physical Chemistry Chemical Physics, 2018, 20, 17847-17858.	1.3	9
141	On the role of dynamic electron correlation in non-orthogonal configuration interaction with fragments. Physical Chemistry Chemical Physics, 2022, 24, 11931-11944.	1.3	9
142	Extraction of Magnetic Coupling Parameters in 2-Dimensional Magnetic Honeycomb Layers. Journal of Physical Chemistry A, 2010, 114, 7553-7560.	1.1	8
143	The Role of Vibrational Anharmonicity in the Computational Study of Thermal Spin Crossover. Magnetochemistry, 2019, 5, 49.	1.0	8
144	GronOR: Scalable and Accelerated Nonorthogonal Configuration Interaction for Molecular Fragment Wave Functions. Journal of Chemical Theory and Computation, 2022, 18, 3549-3565.	2.3	8

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145	Mid-gap excitations in Anderson polyoxometalates. Chemical Physics Letters, 2008, 450, 391-395.	1.2	7
146	Simple versus composite nature of the magnetic coupling in copper and nickel-based metallic chains. Over- and underestimation of J. Comptes Rendus Chimie, 2012, 15, 163-169.	0.2	7
147	Zero-Field Splitting in Transition Metal Complexes: Ab Initio Calculations, Effective Hamiltonians, Model Hamiltonians, and Crystal-Field Models. , 2017, , 765-796.		7
148	Theoretical studies on the energy structures and optical properties of copper cysteamine â€“ a novel sensitizer. Physical Chemistry Chemical Physics, 2019, 21, 21084-21093.	1.3	7
149	Trends in the Bond Multiplicity of Cr₂, Cr₃, and Cr₂M (M = Zn, Ni,) Tj ETQq1 1 0.784314 rgBT Chemistry A, 2019, 123, 1538-1547.	1.1	7
150	Computational study of the staircase molecular conductivity of polyoxovanadates adsorbed on Au(111). Dalton Transactions, 2021, 50, 5540-5551.	1.6	7
151	Theoretical study of the magnetic exchange interaction in catena-Î¼-Tris[oxalato(2-)-O1,O2;O3,O4]-dicopper complex with interlocked helical chains. Chemical Physics, 2011, 379, 109-115.	0.9	6
152	Rationalization of the behavior of M₂(CH₃CS₂)₄I (M) Tj ETQq0 0 0 rgBT /Overlock calculations. Journal of Computational Chemistry, 2012, 33, 1748-1761.	1.5	6
153	Mononuclear and binuclear iron(III) complexes incorporating N4O3 coordinating heptadentate ligand: Synthesis, structure and magnetic properties. Polyhedron, 2008, 27, 2751-2756.	1.0	5
154	Towards a low-spin configuration in extended metal atom chains. Theoretical study of trimetallic systems with 22 metal electrons. Dalton Transactions, 2012, 41, 498-504.	1.6	5
155	Photoinduced Moâ€“CN Bond Breakage in Octacyanomolybdate Leading to Spin Triplet Trapping. Angewandte Chemie, 2020, 132, 3141-3145.	1.6	5
156	Density functional theory study of single-molecule ferroelectricity in Preyssler-type polyoxometalates. APL Materials, 2021, 9, .	2.2	5
157	Quantum dynamics simulations of the thermal and light-induced high-spin to low-spin relaxation in Fe(bpy)₃ and Fe(mtz)₆. Faraday Discussions, 0, 237, 93-107.	1.6	5
158	Quantum molecular dynamic simulation of an excess electron in dense helium. Journal of Chemical Physics, 1992, 97, 408-416.	1.2	4
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