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	Molecular Transition Metal Oxide Electrocatalysts for the Reversible Carbon Dioxideâ€“Carbon Monoxide Transformation. Angewandte Chemie - International Edition, 2022, 61, .	7.2	15
2	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
3	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
4	U₂N@I_h(7)-C₈₀: fullerene cage encapsulating an unsymmetrical U(<scp>iv</scp>)â€“U(<scp>v</scp>) cluster. Chemical Science, 2021, 12, 282-292.	3.7	25
5	Computational study of the staircase molecular conductivity of polyoxovanadates adsorbed on Au(111). Dalton Transactions, 2021, 50, 5540-5551.	1.6	7
6	Density functional theory study of single-molecule ferroelectricity in Preyssler-type polyoxometalates. APL Materials, 2021, 9, .	2.2	5
7	Characterization of a strong covalent Th3+â€“Th3+ bond inside an Ih(7)-C80 fullerene cage. Nature Communications, 2021, 12, 2372.	5.8	34
8	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
9	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
10	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
11	Gating the conductance of extended metal atom chains: a computational analysis of Ru₃(dpa)₄(NCS)₂ and [Ru₃(npa)₄(NCS)₂]. Physical Chemistry Chemical Physics, 2021, 23, 14836-14844.	1.3	0
12	Ultrafast Intersystem Crossing in Xanthone from Wavepacket Dynamics. Journal of the American Chemical Society, 2021, 143, 21474-21477.	6.6	10
13	Photoinduced Moâ€“CN Bond Breakage in Octacyanomolybdate Leading to Spin Triplet Trapping. Angewandte Chemie, 2020, 132, 3141-3145.	1.6	5
14	Photoinduced Moâ€“CN Bond Breakage in Octacyanomolybdate Leading to Spin Triplet Trapping. Angewandte Chemie - International Edition, 2020, 59, 3117-3121.	7.2	30
15	Switchable Rashba anisotropy in layered hybrid organicâ€“inorganic perovskite by hybrid improper ferroelectricity. Npj Computational Materials, 2020, 6, .	3.5	26
16	Controlling the Lifetime of the Triplet MLCT State in Fe(II) Polypyridyl Complexes through Ligand Modification. Inorganics, 2020, 8, 16.	1.2	10
17	GronOR: Massively parallel and GPU-accelerated non-orthogonal configuration interaction for large molecular systems. Journal of Chemical Physics, 2020, 152, 064111.	1.2	20
18	Reduced Common Molecular Orbital Basis for Nonorthogonal Configuration Interaction. Journal of Chemical Theory and Computation, 2020, 16, 2941-2951.	2.3	20

#	Article	IF	Citations
19	Pre-exascale accelerated application development: The ORNL Summit experience. IBM Journal of Research and Development, 2020, 64, 11:1-11:21.	3.2	15
20	Deactivation of Excited States in Transitionâ€Metal Complexes: Insight from Computational Chemistry. Chemistry - A European Journal, 2019, 25, 1152-1164.	1.7	19
21	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
22	The Role of Vibrational Anharmonicity in the Computational Study of Thermal Spin Crossover. Magnetochemistry, 2019, 5, 49.	1.0	8
23	Trends in the Bond Multiplicity of Cr₂, Cr₃, and Cr₂M (M = Zn, Ni,) Tj ETQq1 1 0.784314 rgBT /Overlock Chemistry A, 2019, 123, 1538-1547.	1.1	7
24	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
25	Computer-aided design of short-lived phosphorescent Ru(II) polarity probes. Dyes and Pigments, 2019, 162, 168-176.	2.0	3
26	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
27	Quantum Chemical Study of the Interligand Electron Transfer in Ru Polypyridyl Complexes. Journal of Physical Chemistry A, 2018, 122, 1114-1123.	1.1	9
28	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
29	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
30	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
31	The magnetic fingerprint of dithiazolyl-based molecule magnets. Physical Chemistry Chemical Physics, 2018, 20, 20406-20416.	1.3	16
32	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 /Overlock Physical Chemistry Chemical Physics, 2018, 20, 17847-17858.	1.3	9
33	Quantum Chemical Characterization of Single Molecule Magnets Based on Uranium. Journal of Physical Chemistry A, 2017, 121, 1726-1733.	1.1	25
34	A multiconfigurational approach to the electronic structure of trichromium extended metal atom chains. Dalton Transactions, 2017, 46, 6202-6211.	1.6	10
35	Backbone flexibility of extended metal atom chains. Ab initio molecular dynamics for Cr₃(dpa)₄X₂ (X = NCS, CN, NO₃) in gas and crystalline phases. Dalton Transactions, 2017, 46, 15487-15493.	1.6	4
36	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

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37	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
38	Zero-Field Splitting in Transition Metal Complexes: Ab Initio Calculations, Effective Hamiltonians, Model Hamiltonians, and Crystal-Field Models. , 2017, , 765-796.		7
39	Phenylazopyridine as Switch in Photochemical Reactions. A Detailed Computational Description of the Mechanism of Its Photoisomerization. Materials, 2017, 10, 1342.	1.3	15
40	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
41	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
42	Photoreduction Mechanism of CO₂ to CO Catalyzed by a Rhenium(I)â€“Polyoxometalate Hybrid Compound. ACS Catalysis, 2016, 6, 6422-6428.	5.5	58
43	Amidiniumâ€Containing 2D [MnCr] Dimetallic Oxalateâ€Based Networks â€“ The Influence on Structure and Magnetism Explored by Combining Experience and Theory. European Journal of Inorganic Chemistry, 2016, 2016, 4185-4193.	1.0	4
44	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
45	Towards a Quantitative Understanding. Theoretical Chemistry and Computational Modelling, 2016, , 141-175.	0.2	0
46	Magnetism and Conduction. Theoretical Chemistry and Computational Modelling, 2016, , 177-212.	0.2	0
47	Magnetic Interactions in Molecules and Solids. Theoretical Chemistry and Computational Modelling, 2016, , .	0.2	32
48	Zero-Field Splitting in Transition Metal Complexes: Ab Initio Calculations, Effective Hamiltonians, Model Hamiltonians, and Crystal-Field Models. , 2016, , 1-31.		1
49	Synergy and destructive interferences between local magnetic anisotropies in binuclear complexes. AIP Conference Proceedings, 2015, , .	0.3	0
50	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
51	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
52	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
53	Managing the Computational Chemistry Big Data Problem: The ioChem-BD Platform. Journal of Chemical Information and Modeling, 2015, 55, 95-103.	2.5	403
54	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

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55	Methods for describing open-shell systems: Following the trail of Rosa Caballol's research. International Journal of Quantum Chemistry, 2014, 114, 481-492.	1.0	0
56	Improving the calculation of magnetic coupling constants in MRPT methods. Journal of Computational Chemistry, 2014, 35, 1665-1671.	1.5	20
57	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
58	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
59	Artificial chemical and magnetic structure at the domain walls of an epitaxial oxide. Nature, 2014, 515, 379-383.	13.7	146
60	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
61	Interplay between Local Anisotropies in Binuclear Complexes. Inorganic Chemistry, 2014, 53, 4508-4516.	1.9	36
62	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
63	Computational approach to the study of thermal spin crossover phenomena. Journal of Chemical Physics, 2014, 140, 184318.	1.2	57
64	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
65	Explanation of the site-specific spin crossover in Fe(mtz)6(BF4)2. Dalton Transactions, 2013, 42, 14702.	1.6	15
66	Origin of the Magnetic Anisotropy in Heptacoordinate Ni^{II} and Co^{II} Complexes. Chemistry - A European Journal, 2013, 19, 950-956.	1.7	145
67	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
68	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
69	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
70	H₂Sâ€Mediated Thermal and Photochemical Methane Activation. ChemPhysChem, 2013, 14, 3960-3970.	1.0	9
71	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
72	Magnetic interactions in LiCu2O2: Single-chain versus double-chain models. Physical Review B, 2012, 86, .	1.1	23

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73	The Absorption Spectrum of Cytosine Tautomers: Beyond the Static Approach. Journal of Chemical Theory and Computation, 2012, 8, 235-244.	2.3	29
74	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
75	Metal-to-metal charge-transfer transitions: reliable excitation energies from ab initio calculations. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	31
76	First-principles study of magnetic interactions in cupric oxide. Physical Review B, 2012, 85, .	1.1	26
77	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
78	Rationalization of the behavior of M₂(CH₃CS₂)₄I (M) Tj ETQq0 0 0 rgBT /Overlock 1 calculations. Journal of Computational Chemistry, 2012, 33, 1748-1761.	1.5	6
79	The electronic structure of Ullman's biradicals: an orthogonal valence bond interpretation. Physical Chemistry Chemical Physics, 2011, 13, 14617.	1.3	24
80	Insights on the photomagnetism in copper octacyanomolybdates. Dalton Transactions, 2011, 40, 7295.	1.6	29
81	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
82	Theoretical Determination of the Zero-Field Splitting in Copper Acetate Monohydrate. Inorganic Chemistry, 2011, 50, 6229-6236.	1.9	91
83	Analysis of the magnetic coupling in nitroxide organic biradicals. Theoretical Chemistry Accounts, 2011, 128, 505-519.	0.5	31
84	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
85	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
86	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
87	Spin crossover in Fe(II) complexes: An ab initio study of ligand Ïƒâ€donation. International Journal of Quantum Chemistry, 2010, 110, 331-337.	1.0	46
88	Isotropic Non-Heisenberg Behavior in M₃(dpa)₄Cl₂ Extended Metal Atom Chains. Journal of Physical Chemistry A, 2010, 114, 12291-12298.	1.1	14
89	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
90	Rigorous Extraction of the Anisotropic Multispin Hamiltonian in Bimetallic Complexes from the Exact Electronic Hamiltonian. Journal of Chemical Theory and Computation, 2010, 6, 977-977.	2.3	2

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91	Analysis of the Magnetic Coupling in M₃(dpa)₄Cl₂Systems (M = Ni,) Tj ETQq1 1 0.784314 rgBT	1.1	21
92	Extraction of Magnetic Coupling Parameters in 2-Dimensional Magnetic Honeycomb Layers. Journal of Physical Chemistry A, 2010, 114, 7553-7560.	1.1	8
93	Antisymmetric Magnetic Interactions in Oxo-Bridged Copper(II) Bimetallic Systems. Journal of Chemical Theory and Computation, 2010, 6, 3092-3101.	2.3	51
94	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
95	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
96	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
97	On the mechanism of the photoinduced magnetism in copper octacyanomolybdates. Chemical Communications, 2010, 46, 5737.	2.2	30
98	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
99	Energetics of [Fe(NCH)₆]²⁺ via CASPT2 calculations: A spinâ€crossover perspective. Journal of Computational Chemistry, 2009, 30, 2327-2333.	1.5	61
100	Ab initio study of the singlet-triplet splitting in reduced polyoxometalates. Theoretical Chemistry Accounts, 2009, 123, 3-10.	0.5	18
101	Ferromagnetism and increased ionicity in epitaxially grownTbMnO3films. Physical Review B, 2009, 79, .	1.1	58
102	Universal Theoretical Approach to Extract Anisotropic Spin Hamiltonians. Journal of Chemical Theory and Computation, 2009, 5, 2977-2984.	2.3	270
103	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
104	Mononuclear and binuclear iron(III) complexes incorporating N4O3 coordinating heptadentate ligand: Synthesis, structure and magnetic properties. Polyhedron, 2008, 27, 2751-2756.	1.0	5
105	Mid-gap excitations in Anderson polyoxometalates. Chemical Physics Letters, 2008, 450, 391-395.	1.2	7
106	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
107	On the Heisenberg behaviour of magnetic coupling in the manganese dimer. Chemical Physics Letters, 2008, 458, 290-294.	1.2	31
108	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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109	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
110	Embedded Cluster Approach: 3d Perovskite Oxides. , 2008, , 1-6.		0
111	Isotropic non-Heisenberg terms in the magnetic coupling of transition metal complexes. Journal of Chemical Physics, 2008, 129, 104102.	1.2	43
112	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
113	Renormalization of quasiparticle hopping integrals by spin interactions in layered copper oxides. Physical Review B, 2007, 75, .	1.1	9
114	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
115	Polyoxometalates with Internal Cavities:â€‰ Redox Activity, Basicity, and Cation Encapsulation in [Xⁿ⁺P₅W₃₀O₁₁₀]⁽¹⁵⁻ⁿ Preyssler Complexes, with X = Na⁺, Ca²⁺, Y³⁺, La³⁺, Ce³⁺, and Th⁴⁺. Journal of the American Chemical Society, 2007, 129, 12244-12253.	6.6	152
116	Role of charge transfer configurations in LaMnO3, CaMnO3, and CaFeO3. Journal of Chemical Physics, 2007, 126, 134709.	1.2	38
117	Many-Electron Bands in Transition Metal Compounds. AIP Conference Proceedings, 2007, , .	0.3	0
118	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
119	Ab initiostudy of the Zener polaron spectrum of half-doped manganites: Comparison of several model Hamiltonians. Physical Review B, 2006, 74, .	1.1	14
120	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
121	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
122	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
123	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
124	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
125	Ni 3s-hole states in NiO by non-orthogonal configuration interaction. Chemical Physics, 2006, 331, 178-185.	0.9	13
126	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

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127	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
128	Toward a variational treatment of the magnetic coupling between centers with elevated spin moments. Chemical Physics, 2005, 309, 259-269.	0.9	31
129	Electronic structure ofCaCu2O3: Spin ladder versus one-dimensional spin chain. Physical Review B, 2005, 71, .	1.1	29
130	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
131	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
132	Ab initiotheory of magnetic interactions at surfaces. Journal of Physics Condensed Matter, 2004, 16, S2557-S2574.	0.7	11
133	Magnetic interactions in calcium and sodium ladder vanadates. Journal of Chemical Physics, 2004, 120, 961-967.	1.2	26
134	Ab initiostudy of the charge order and Zener polaron formation in half-doped manganites. Physical Review B, 2004, 70, .	1.1	17
135	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
136	Unexpected role of Madelung potential in monoplanar high-Tc cuprate superconductors. Chemical Physics Letters, 2003, 379, 291-296.	1.2	9
137	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
138	Magnetic coupling in oxalato-bridged hetero-bimetallic compounds: an ab initio study. Polyhedron, 2003, 22, 2409-2414.	1.0	12
139	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
140	Electronic structureÎ±â€²â^'NaV2O5:Wave-function-based embedded-cluster calculations. Physical Review B, 2003, 67, .	1.1	22
141	Four-spin cyclic exchange in spin ladder cuprates. Physical Review B, 2003, 67, .	1.1	59
142	Theoretical Characterization of the Ground and Optically Excited States ofÎ±â€²â^'NaV2O5. Physical Review Letters, 2002, 89, 076407.	2.9	27
143	Magnetic structure ofLi2CuO2:â€ƒFromab initiocalculations to macroscopic simulations. Physical Review B, 2002, 66, .	1.1	57
144	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

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145	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
146	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
147	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
148	A relationship between electronic structure effective parameters and Tc in monolayered cuprate superconductors. Chemical Physics Letters, 2001, 345, 183-188.	1.2	16
149	Optical properties of peroxy radicals in silica: Multiconfigurational perturbation theory calculations. Journal of Chemical Physics, 2001, 114, 6259-6264.	1.2	31
150	Stability and optical properties of silver atoms in KCl. Radiation Effects and Defects in Solids, 2001, 154, 249-253.	0.4	0
151	Detailed ab-initio analysis of the magnetic coupling in CuF2. Chemical Physics Letters, 2000, 319, 625-630.	1.2	37
152	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
153	Magnitude of the First and Second Neighbour Magnetic Interactions in the Spin Chain Compound Li2CuO2. International Journal of Molecular Sciences, 2000, 1, 28-38.	1.8	4
154	Neutral atoms in ionic lattices:â€ƒExcited states ofKCl:Ag0. Physical Review B, 2000, 62, 13366-13375.	1.1	18
155	Electronic structure and magnetic interactions of the spin-chain compoundsCa2CuO3andSr2CuO3. Physical Review B, 2000, 63, .	1.1	56
156	Midinfrared spectrum of undoped cuprates:â€ƒd-dtransitions studied byab initiomethods. Physical Review B, 2000, 62, 702-709.	1.1	41
157	Neutral atoms in ionic lattices:â€ƒStability and ground-state properties ofKCl:Ag0. Physical Review B, 2000, 62, 13356-13365.	1.1	12
158	Electric field effects on the ionic-neutral curve crossing of alkali halide molecules. Journal of Chemical Physics, 2000, 113, 9940-9947.	1.2	20
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