Rosa Caballol

List of Publications by Year
in descending order

82 papers	4,154 citations	159573 30 h-index	110368 64 g-index
84 all docs	84 docs citations	84 times ranked	2177 citing authors

#	Article	IF	Citations
1	Quantum Chemical Study of the Interligand Electron Transfer in Ru Polypyridyl Complexes. Journal of Physical Chemistry A, 2018, 122, 1114-1123.	2.5	9
2	Role of the Imide Axial Ligand in the Spin and Oxidation State of Manganese Corrole and Corrolazine Complexes. Inorganic Chemistry, 2016, 55, 5274-5280.	4.0	17
3	Spin-crossover in phenylazopyridine-functionalized Niâ€“porphyrin: transâ€“cis isomerization triggered by Ï€â€“Ï€ interactions. Physical Chemistry Chemical Physics, 2015, 17, 217-225.	2.8	17
4	Electronic structure aspects of the complete O₂ transfer reaction between Ni(<scp>ii</scp>) and Mn(<scp>ii</scp>) complexes with cyclam ligands. Physical Chemistry Chemical Physics, 2015, 17, 2814-2822.	2.8	5
5	Magnetic Interactions in Molecules and Highly Correlated Materials: Physical Content, Analytical Derivation, and Rigorous Extraction of Magnetic Hamiltonians. Chemical Reviews, 2014, 114, 429-492.	47.7	342
6	On the Reaction Mechanism of the Complete Intermolecular O₂ Transfer between Mononuclear Nickel and Manganese Complexes with Macrocyclic Ligands. Chemistry - A European Journal, 2014, 20, 13296-13304.	3.3	7
7	The role of macrocyclic ligands in the peroxo/superoxo nature of Niâ€“O₂ biomimetic complexes. Journal of Computational Chemistry, 2012, 33, 1407-1415.	3.3	13
8	Comparing the peroxo/superoxo nature of the interaction between molecular O2 and Î²-diketiminato-copper and nickel complexes. Physical Chemistry Chemical Physics, 2011, 13, 20241.	2.8	30
9	The electronic structure of Ullman's biradicals: an orthogonal valence bond interpretation. Physical Chemistry Chemical Physics, 2011, 13, 14617.	2.8	24
10	Insights on the photomagnetism in copper octacyanomolybdates. Dalton Transactions, 2011, 40, 7295.	3.3	29
11	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.	2.4	16
12	Analysis of the magnetic coupling in nitroxide organic biradicals. Theoretical Chemistry Accounts, 2011, 128, 505-519.	1.4	31
13	Electronic structure and relative stability of 1:1 Cuâ€“O₂ adducts from differenceâ€dedicated configuration interaction calculations. Journal of Computational Chemistry, 2011, 32, 1144-1158.	3.3	20
14	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.	1.9	6
15	Extending the active space in multireference configuration interaction calculations of magnetic coupling constants. Theoretical Chemistry Accounts, 2010, 126, 185-196.	1.4	24
16	Extraction of Magnetic Coupling Parameters in 2-Dimensional Magnetic Honeycomb Layers. Journal of Physical Chemistry A, 2010, 114, 7553-7560.	2.5	8
17	Analysis of the magnetic coupling in binuclear systems. III. The role of the ligand to metal charge transfer excitations revisited. Journal of Chemical Physics, 2009, 131, 044327.	3.0	110
18	Ab initio study of the singlet-triplet splitting in reduced polyoxometalates. Theoretical Chemistry Accounts, 2009, 123, 3-10.	1.4	18

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19	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.	3.3	84
20	On the Heisenberg behaviour of magnetic coupling in the manganese dimer. Chemical Physics Letters, 2008, 458, 290-294.	2.6	31
21	Accurate Determination of the Electronic Structure Parameters of the Spin Ladder Compounds SrCu2O3, Sr2Cu3O5 and CaCu2O3. Theoretical Chemistry Accounts, 2006, 116, 535-548.	1.4	10
22	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
23	Toward a variational treatment of the magnetic coupling between centers with elevated spin moments. Chemical Physics, 2005, 309, 259-269.	1.9	31
24	Electronic structure ofCaCu2O3: Spin ladder versus one-dimensional spin chain. Physical Review B, 2005, 71, .	3.2	29
25	Ab initio study of the singletâ€“triplet relative stability of 2,6-dibromo-2â€²,6â€²-bistrifluoromethyl-diphenylmethylene. Chemical Physics, 2004, 303, 157-164.	1.9	3
26	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.	3.3	80
27	Magnetic coupling in oxalato-bridged hetero-bimetallic compounds: an ab initio study. Polyhedron, 2003, 22, 2409-2414.	2.2	12
28	Ferrimagnetic coupling in oxamido-bridged Mn(II)Cu(II) compounds: a combined CASPT2 and DDCI study. Molecular Physics, 2003, 101, 2095-2102.	1.7	17
29	Four-spin cyclic exchange in spin ladder cuprates. Physical Review B, 2003, 67, .	3.2	59
30	Analysis of the magnetic coupling in binuclear complexes. II. Derivation of valence effective Hamiltonians from ab initio CI and DFT calculations. Journal of Chemical Physics, 2002, 116, 3985-4000.	3.0	213
31	Metalâ^'Ligand Delocalization in Magnetic Orbitals of Binuclear Complexes. Journal of Physical Chemistry A, 2002, 106, 8146-8155.	2.5	84
32	Derivation of spin Hamiltonians from the exact Hamiltonian: Application to systems with two unpaired electrons per magnetic site. Physical Review B, 2002, 66, .	3.2	60
33	Efficiency of a controlled use of Davidson's correction for the calculation of excitation energies: vertical spectrum oftrans-butadiene. Molecular Physics, 2002, 100, 919-926.	1.7	18
34	Analysis of the magnetic coupling in binuclear complexes. I. Physics of the coupling. Journal of Chemical Physics, 2002, 116, 2728-2747.	3.0	272
35	Excitation Energy Dedicated Molecular Orbitals. Method and Applications to Magnetic Systems. Journal of Physical Chemistry A, 2000, 104, 11636-11643.	2.5	36
36	Ab Initio Study of the Exchange Coupling in Oxalato-Bridged Cu(II) Dinuclear Complexes. Journal of Physical Chemistry A, 2000, 104, 9983-9989.	2.5	103

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37	The Controversial Ground State of Tetramethyleneethane. An ab Initio CI Study. Journal of Physical Chemistry A, 2000, 104, 6253-6258.	2.5	41
38	Singletâ^'Triplet Gap in Î±-n-Dehydrotoluene and Related Biradicals:Â An ab Initio Configuration Interaction Study. Journal of Physical Chemistry A, 1999, 103, 6220-6224.	2.5	26
39	Ab Initio Configuration Interaction Calculation of the Exchange Coupling Constant in Hydroxo Doubly Bridged Cr(III) Dimers. Inorganic Chemistry, 1999, 38, 668-673.	4.0	65
40	Dedicated Molecular Orbitals for the Variational Determination of the Electron-Transfer Matrix Element. Method and Application to a Cu(I)â^'Cu(II) Mixed Valence Compound. Journal of Physical Chemistry A, 1997, 101, 1716-1721.	2.5	19
41	Remarks on the Proper Use of the Broken Symmetry Approach to Magnetic Coupling. Journal of Physical Chemistry A, 1997, 101, 7860-7866.	2.5	421
42	Application of the iterative difference-dedicated configuration interaction method to the determination of excitation energies in some benchmark systems: Be, CH + , BH and CH 2. Theoretical Chemistry Accounts, 1997, 98, 50-56.	1.4	25
43	Calculation of small transition energies from a dressed configuration interaction. Chemical Physics Letters, 1997, 265, 621-628.	2.6	15
44	On the quasidiabatic character of average natural orbitals. Chemical Physics Letters, 1997, 281, 161-167.	2.6	28
45	Ab InitioCI Determination of the Exchange Coupling Constant of Doubly-Bridged Nickel(II) Dimers. Inorganic Chemistry, 1996, 35, 1609-1615.	4.0	75
46	A general bridge between configuration interaction and coupled-cluster methods: a multistate solution. Chemical Physics Letters, 1996, 259, 619-626.	2.6	7
47	Theoretical study of the ethylene electronic spectrum and extraction of an r-dependent Hubbard Hamiltonian. Chemical Physics Letters, 1996, 261, 98-104.	2.6	36
48	Stateâ€specific coupled clusterâ€type dressing of multireference singles and doubles configuration interaction matrix. Journal of Chemical Physics, 1996, 104, 4068-4076.	3.0	75
49	An iterative difference-dedicated configuration interaction. Proposal and test studies. Chemical Physics Letters, 1995, 238, 222-229.	2.6	125
50	Ab Initio Study of Ullman's Nitroxide Biradicals. Exchange Coupling versus Structural Characteristics Analysis. The Journal of Physical Chemistry, 1995, 99, 154-157.	2.9	52
51	Multireference selfâ€consistent sizeâ€consistent singles and doubles configuration interaction for ground and excited states. Journal of Chemical Physics, 1994, 101, 8908-8921.	3.0	78
52	Towards anAb InitioDescription of Magnetism in Ionic Solids. Physical Review Letters, 1994, 72, 2669-2669.	7.8	0
53	The full-CI energy of the NH3 molecule in a DZP basis set. Chemical Physics Letters, 1994, 218, 283-286.	2.6	8
54	Structural dependence of the singlet-triplet gap in doubly bridged copper dimers: a variational CI calculation. Chemical Physics, 1994, 179, 377-384.	1.9	61

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55	Size-consistent selected configuration interaction calculations. A few tests of efficiency. Chemical Physics Letters, 1993, 209, 126-134.	2.6	18
56	Specific CI calculation of energy differences: Transition energies and bond energies. Chemical Physics, 1993, 172, 33-43.	1.9	412
57	Towards anab initiodescription of magnetism in ionic solids. Physical Review Letters, 1993, 71, 3549-3552.	7.8	69
58	Variational calculation of small energy differences. The singlet-triplet gap in [Cu2Cl6]2â^'. Chemical Physics Letters, 1992, 198, 555-562.	2.6	281
59	Direct selected configuration interaction using a hole-particle formalism. Chemical Physics Letters, 1992, 188, 543-549.	2.6	37
60	Observable-dedicated molecular orbitals. I. Method and illustrations. Chemical Physics, 1991, 153, 25-37.	1.9	38
61	Ab initio CI calculations on ScC2H4+ ions. Chemical Physics Letters, 1990, 167, 421-428.	2.6	4
62	Improved non-valence virtual orbitals for CI calculations. Chemical Physics, 1990, 140, 7-18.	1.9	12
63	Theoretical analysis of the rearrangement and inversion processes in oxiranyl radicals. Computational and Theoretical Chemistry, 1988, 168, 93-104.	1.5	1
64	Unimolecular reactions of the enolic tautomer of ionized acetic acid in the gas phase: an ab initio and RRKM study. The Journal of Physical Chemistry, 1988, 92, 3336-3341.	2.9	6
65	Ab initio study of stable bis(carbon dioxide)molybdenum complexes. Journal of the Chemical Society Dalton Transactions, 1987, , 2373.	1.1	9
66	Reactivity of pyrrole pigments. Part 9 MINDO/3 calculations on dipyrrolic partial models of bile pigments. Monatshefte FÃ¼r Chemie, 1987, 118, 993-1010.	1.8	7
67	Reactivity of pyrrole pigments. Part 10 MINDO/3 calculations on bile pigments. Monatshefte FÃ¼r Chemie, 1987, 118, 1011-1029.	1.8	6
68	The hydrogen bonding in H3Yâ€¦HX (Y=P, As; X=Cl, Br) complexes: An ab initio CI study. Chemical Physics Letters, 1987, 141, 334-338.	2.6	6
69	Theoretical study of the different coordination modes of copper-carbon dioxide complex. The Journal of Physical Chemistry, 1987, 91, 1328-1333.	2.9	63
70	Theoretical study on the isomerization and dissociation of C4H4O+? radical cation. Journal of the Chemical Society Perkin Transactions II, 1986, , 949.	0.9	3
71	Jahn-teller distortions in XH4+ radical cations (X = Si, Ge, Sn). an ab initio CI study. Chemical Physics Letters, 1986, 130, 278-284.	2.6	27
72	Theoretical analysis of the isomerizations and fragmentations of the C3H6O2+Â· radical cation. International Journal of Mass Spectrometry and Ion Processes, 1986, 71, 75-84.	1.8	5

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73	Phenol cation dissociation: theoretical study of the potential surface and RRKM statistical analysis. The Journal of Physical Chemistry, 1985, 89, 5836-5840.	2.9	7
74	MINDO/3 potential energy surface for hydrogen-graphite system: Active sites and migration. Surface Science, 1985, 149, 621-629.	1.9	22
75	On the isomerization and dissociation reactions of C4H4O radical cation. Computational and Theoretical Chemistry, 1985, 122, 281-285.	1.5	2
76	Theoretical interstellar and prebiotic organic chemistry: A tentative methodology. Origins of Life and Evolution of Biospheres, 1976, 7, 163-173.	0.6	1
77	Extended HÃ¼ckel theory of hydrogen-molecule interactions. International Journal of Quantum Chemistry, 1975, 9, 1021-1031.	2.0	2
78	All valence electron wavefunctions and electrostatic molecular potentials under zero differential overlap approximation. Chemical Physics Letters, 1974, 25, 89-91.	2.6	17
79	Ground and first excited states electrostatic molecular potentials of ketene and diazomethane. Chemical Physics Letters, 1974, 28, 422-426.	2.6	10
80	Generalized open shell SCF theory. International Journal of Quantum Chemistry, 1974, 8, 373-394.	2.0	45
81	Ã‰tude conformationnelle dâ€™Ã©thylamines polychlorÃ©es. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1974, 71, 295-297.	0.2	2
82	Analyse conformationnelle de la glycine. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1973, 70, 154-159.	0.2	1