IbÃ©rio De P R Moreira

List of Publications by Year
in descending order

94 papers	4,402 citations	101543 36 h-index	106344 65 g-index
99 all docs	99 docs citations	99 times ranked	3746 citing authors

#	Article	IF	Citations
1	Controlling Chemical Reactivity with Optimally Oriented Electric Fields: A Generalization of the Newton Trajectory Method. Journal of Chemical Theory and Computation, 2022, 18, 935-952.	5.3	6
2	Electronic structure and magnetic coupling in selenium substituted pyridine-bridged bisdithiazolyl multifunctional molecular materials. Physical Chemistry Chemical Physics, 2022, 24, 12196-12207.	2.8	2
3	2D Hexagonal Covalent Organic Radical Frameworks as Tunable Correlated Electron Systems. Advanced Functional Materials, 2021, 31, 2004584.	14.9	14
4	Controlling pairing of Ï€-conjugated electrons in 2D covalent organic radical frameworks via in-plane strain. Nature Communications, 2021, 12, 1705.	12.8	18
5	Quantum equilibration of the double-proton transfer in a model system porphine. Physical Chemistry Chemical Physics, 2020, 22, 22332-22341.	2.8	0
6	Quantum Zermelo problem for general energy resource bounds. Physical Review Research, 2020, 2, .	3.6	2
7	Interplay between the Gentlest Ascent Dynamics Method and Conjugate Directions to Locate Transition States. Journal of Chemical Theory and Computation, 2019, 15, 5426-5439.	5.3	3
8	Post-B3LYP Functionals Do Not Improve the Description of Magnetic Coupling in Cu(II) Dinuclear Complexes. Journal of Physical Chemistry A, 2018, 122, 3423-3432.	2.5	12
9	A 2D rhomboidal system of manganese(<scp>ii</scp>) [Mn(3-MeC₆H₄COO)₂(H₂O)₂]_n with spin canting: rationalization of the magnetic exchange. Dalton Transactions, 2018, 47, 3717-3724.	3.3	6
10	Exploring potential energy surfaces with gentlest ascent dynamics in combination with the shrinking dimer method and Newtonian dynamics. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	3
11	Redox-Induced Gating of the Exchange Interactions in a Single Organic Diradical. ACS Nano, 2017, 11, 5879-5883.	14.6	50
12	Experimental and Computational Evidence of the Biradical Structure and Reactivity of Titanium(IV) Enolates. Journal of Organic Chemistry, 2017, 82, 8909-8916.	3.2	10
13	Calix[n]arene-based polyradicals: enhancing ferromagnetism by avoiding edge effects. Physical Chemistry Chemical Physics, 2017, 19, 24264-24270.	2.8	6
14	Existence of multi-radical and closed-shell semiconducting states in post-graphene organic Dirac materials. Nature Communications, 2017, 8, 1957.	12.8	45
15	Design of multi-functional 2D open-shell organic networks with mechanically controllable properties. Chemical Science, 2017, 8, 1027-1039.	7.4	16
16	Helical Folding-Induced Stabilization of Ferromagnetic Polyradicals Based on Triarylmethyl Radical Derivatives. Journal of the American Chemical Society, 2016, 138, 5271-5275.	13.7	11
17	Magnetic Coupling Constants in Three Electrons Three Centers Problems from Effective Hamiltonian Theory and Validation of Broken Symmetry-Based Approaches. Journal of Chemical Theory and Computation, 2016, 12, 3228-3235.	5.3	14
18	Exchange Coupling Inversion in a High-Spin Organic Triradical Molecule. Nano Letters, 2016, 16, 2066-2071.	9.1	60

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19	Formylation of Electron-Rich Aromatic Rings Mediated by Dichloromethyl Methyl Ether and TiCl4: Scope and Limitations. Molecules, 2015, 20, 5409-5422.	3.8	20
20	Spin Adapted versus Broken Symmetry Approaches in the Description of Magnetic Coupling in Heterodinuclear Complexes. Journal of Chemical Theory and Computation, 2015, 11, 1006-1019.	5.3	14
21	Tripletâ€“singlet gap in structurally flexible organic diradicals. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	7
22	Handling Magnetic Coupling in Trinuclear Cu(II) Complexes. Journal of Chemical Theory and Computation, 2015, 11, 3650-3660.	5.3	13
23	On the Mechanism of Phenolic Formylation Mediated by TiCl₄ Complexes: Existence of Diradical Intermediates Induced by Valence Tautomerism. European Journal of Organic Chemistry, 2015, 2015, 2111-2118.	2.4	4
24	Electronic Structure and Magnetic Properties of CuFeS₂. Inorganic Chemistry, 2015, 54, 4840-4849.	4.0	69
25	The Tripletâ€“Singlet Gap in the m-Xylylene Radical: A Not So Simple One. Journal of Chemical Theory and Computation, 2014, 10, 335-345.	5.3	56
26	Nature of Holes, Oxidation States, and Hypervalency in Covellite (CuS). Inorganic Chemistry, 2014, 53, 12402-12406.	4.0	68
27	Remarks on the exact energy functional for fermions: an analysis using the LÃ¶wdin partitioningÂtechnique. Molecular Physics, 2014, 112, 809-817.	1.7	1
28	Theoretical and computational investigation of meta-phenylene as ferromagnetic coupler in nitronyl nitroxide diradicals. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	12
29	Hetero triply-bridged dinuclear copper(<scp>ii</scp>) compounds with ferromagnetic coupling: a challenge for current density functionals. Physical Chemistry Chemical Physics, 2013, 15, 1966-1975.	2.8	21
30	A comparison model between density functional and wave function theories by means of the LÃ¶wdin partitioning technique. Journal of Chemical Physics, 2013, 138, 174107.	3.0	5
31	General model for explicitly hole-doped superconductor parent compounds: Electronic structure of Ca<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>Na<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>CuO<mml:math xmlns:mml="http://www.w3.org/1998/M	3.0	5
32	Disruption of the Chemical Environment and Electronic Structure in p-Type Cu₂O Films by Alkaline Doping. Journal of Physical Chemistry C, 2012, 116, 13524-13535.	3.1	18
33	Electronic, structural, and optical properties of host materials for inorganic phosphors. Journal of Alloys and Compounds, 2012, 513, 630-640.	5.5	27
34	New Series of Triply Bridged Dinuclear Cu(II) Compounds: Synthesis, Crystal Structure, Magnetic Properties, and Theoretical Study. Inorganic Chemistry, 2011, 50, 10648-10659.	4.0	31
35	Electronic structure of HgBa2Canâ^’1CunO2n+2 (n = 1, 2, 3) superconductor parent compounds from periodic hybrid density functional theory. Journal of Chemical Physics, 2011, 134, 074709.	3.0	12
36	Electronic and magnetic structure of bulk cobalt: The Î±, Î², and Îµ-phases from density functional theory calculations. Journal of Chemical Physics, 2010, 133, 024701.	3.0	83

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37	Differential Behavior of Aminoâ€“Imino Constitutional Isomers in Nonlinear Optical Processes. ChemPhysChem, 2010, 11, 912-919.	2.1	5
38	Electronic structure of single-layered undoped cuprates from hybrid density functional theory. Physical Review B, 2010, 81, .	3.2	34
39	Toward the Design of Ferromagnetic Molecular Complexes: Magnetostructural Correlations in Ferromagnetic Triply Bridged Dinuclear Cu(II) Compounds Containing Carboxylato and Hydroxo Bridges. Inorganic Chemistry, 2010, 49, 285-294.	4.0	30
40	Description of magnetic interactions in strongly correlated solids via range-separated hybrid functionals. Physical Review B, 2009, 79, .	3.2	44
41	Performance of planeâ€waveâ€based LDA+U and GGA+U approaches to describe magnetic coupling in molecular systems. Journal of Computational Chemistry, 2009, 30, 2316-2326.	3.3	35
42	Electronic Structure and Magnetic Properties of Potassium Ozonide KO3. Inorganic Chemistry, 2009, 48, 5938-5945.	4.0	9
43	Chemical Bonding and Electronic and Magnetic Structure in LaOFeAs. Journal of the American Chemical Society, 2009, 131, 906-907.	13.7	15
44	Periodic density functional theory study of spin crossover in the cesium iron hexacyanochromate prussian blue analog. Journal of Chemical Physics, 2009, 130, 014702.	3.0	13
45	Approaching nanoscale oxides: models and theoretical methods. Chemical Society Reviews, 2009, 38, 2657.	38.1	105
46	Prediction of half-metallic conductivity in Prussian Blue derivatives. Journal of Materials Chemistry, 2009, 19, 2032.	6.7	41
47	Evidence of magnetic ordering of paramagnetic surface defects on partially hydroxylated MgO nanocrystals. Chemical Physics Letters, 2008, 462, 78-83.	2.6	12
48	On the prediction of the crystal and electronic structure of mixed-valence materials by periodic density functional calculations: The case of Prussian Blue. Journal of Chemical Physics, 2008, 128, 044713.	3.0	35
49	Unconventional Biradical Character of Titanium Enolates. Journal of the American Chemical Society, 2008, 130, 3242-3243.	13.7	46
50	Reliability of range-separated hybrid functionals for describing magnetic coupling in molecular systems. Journal of Chemical Physics, 2008, 129, 184110.	3.0	74
51	Performance of the M06 family of exchange-correlation functionals for predicting magnetic coupling in organic and inorganic molecules. Journal of Chemical Physics, 2008, 128, 114103.	3.0	208
52	Spin Hamiltonian effective parameters from periodic electronic structure calculations. Journal of Physics: Conference Series, 2008, 117, 012025.	0.4	12
53	A general procedure to evaluate many-body spin operator amplitudes from periodic calculations: application to cuprates. New Journal of Physics, 2007, 9, 369-369.	2.9	17
54	Restricted Ensemble-Referenced Kohnâ^'Sham versus Broken Symmetry Approaches in Density Functional Theory:â€‰ Magnetic Coupling in Cu Binuclear Complexes. Journal of Chemical Theory and Computation, 2007, 3, 764-774.	5.3	113

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55	Merging multiconfigurational wavefunctions and correlation functionals to predict magnetic coupling constants. Journal of Computational Chemistry, 2007, 28, 2559-2568.	3.3	9
56	The effect of cation coordination on the properties of oxygen vacancies in FeSbO4. Journal of Materials Chemistry, 2006, 16, 1943.	6.7	19
57	A unified view of the theoretical description of magnetic coupling in molecular chemistry and solid state physics. Physical Chemistry Chemical Physics, 2006, 8, 1645.	2.8	200
58	Spin Symmetry Requirements in Density Functional Theory: The Proper Way to Predict Magnetic Coupling Constants in Molecules and Solids. Theoretical Chemistry Accounts, 2006, 116, 587-597.	1.4	77
59	First-Principles Periodic Calculation of Four-Body Spin Terms in High-TcCuprate Superconductors. Physical Review Letters, 2006, 97, 087003.	7.8	23
60	Importance of the embedding environment on the strain within small rings in siliceous materials. Physical Review B, 2006, 73, .	3.2	19
61	Comment on â€œAbout the calculation of exchange coupling constants using density-functional theory: The role of the self-interaction errorâ€•[J. Chem. Phys. 123, 164110 (2005)]. Journal of Chemical Physics, 2006, 124, 107101.	3.0	99
62	On the interplay between inner and outer Krylov spaces applied to large matrix diagonalization algorithms. Computational and Theoretical Chemistry, 2005, 727, 9-19.	1.5	2
63	Magnitude of interplane effective parameters in multilayered high-Tccuprate superconductors. Physical Review B, 2005, 71, .	3.2	9
64	Extent and limitations of density-functional theory in describing magnetic systems. Physical Review B, 2004, 70, .	3.2	122
65	Periodic approach to the electronic structure and magnetic coupling in KCuF3, K2CuF4, and Sr2CuO2Cl2 low-dimensional magnetic systems. International Journal of Quantum Chemistry, 2004, 99, 805-823.	2.0	36
66	Unexpected role of Madelung potential in monoplanar high-Tc cuprate superconductors. Chemical Physics Letters, 2003, 379, 291-296.	2.6	9
67	Ab initioperiodic approach to electronic structure and magnetic exchange inA2CuO2X2(A=Ca,Sr) Tj ETQq1 1 0.784314 rgBT /Overloc	3.2	10
68	Effectivet-Jmodel Hamiltonian parameters of monolayered cuprate superconductors fromab initioelectronic structure calculations. Physical Review B, 2002, 65, .	3.2	50
69	Magnetic structure ofLi2CuO2:â€ƒFromab initiocalculations to macroscopic simulations. Physical Review B, 2002, 66, .	3.2	57
70	Effect of Fock exchange on the electronic structure and magnetic coupling in NiO. Physical Review B, 2002, 65, .	3.2	360
71	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
72	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.	2.5	129

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73	Charge Density Analysis of Triplet and Broken Symmetry States Relevant to Magnetic Coupling in Systems with Localized Spin Moments. Journal of Physical Chemistry A, 2001, 105, 3570-3577.	2.5	37
74	The structural relaxation of the Î±-Al2O3(0001) â€“ an investigation of potential errors. Chemical Physics Letters, 2001, 341, 412-418.	2.6	54
75	A relationship between electronic structure effective parameters and Tc in monolayered cuprate superconductors. Chemical Physics Letters, 2001, 345, 183-188.	2.6	16
76	Accurate and efficient determination of higher roots in diagonalization of large matrices based in function restricted optimization algorithms. Journal of Computational Chemistry, 2000, 21, 1375-1386.	3.3	9
77	Large-scale matrix diagonalization methods by direct optimization of Taylor expansion of Rayleighâ€“Ritz quotient up to third order. Chemical Physics Letters, 2000, 329, 160-167.	2.6	2
78	Detailed ab-initio analysis of the magnetic coupling in CuF2. Chemical Physics Letters, 2000, 319, 625-630.	2.6	37
79	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.	1.4	268
80	Magnitude of the First and Second Neighbour Magnetic Interactions in the Spin Chain Compound Li2CuO2. International Journal of Molecular Sciences, 2000, 1, 28-38.	4.1	4
81	Ab initiostudy ofMF2(M=Mn,Fe,Co,Ni)rutile-type compounds using the periodic unrestricted Hartree-Fock approach. Physical Review B, 2000, 62, 7816-7823.	3.2	46
82	Accurate Prediction of Large Antiferromagnetic Interactions in High-TcHgBa2Canâ^'1CunO2n+2+Î´(n=2,3) Superconductor Parent Compounds. Physical Review Letters, 2000, 84, 1579-1582.	7.8	111
83	Foundations of AB Initio Theory and Applications to Chemisorption and Bulk Properties using the Cluster Model Approach. , 2000, , 129-154.		0
84	Local character of magnetic coupling in ionic solids. Physical Review B, 1999, 59, R6593-R6596.	3.2	117
85	Ab initiostudy of magnetic interactions inKCuF3andK2CuF4low-dimensional systems. Physical Review B, 1999, 60, 5179-5185.	3.2	35
86	Ab initiostudy of the magnetic interactions in the spin-ladder compoundSrCu2O3. Physical Review B, 1999, 60, 3457-3464.	3.2	60
87	Magnetic coupling in the weak ferromagnetCuF2. Physical Review B, 1999, 59, 1016-1023.	3.2	36
88	Through-bond and through-space effects in the magnetic properties of nitroxide biradicals by an integrated QM/MM approach including solvent effects. Chemical Physics Letters, 1999, 302, 240-248.	2.6	40
89	Performance of simplified G2 model chemistry approaches in the study of unimolecular mechanisms: thermal decomposition of acetic acid in gas phase. Computational and Theoretical Chemistry, 1999, 466, 119-126.	1.5	15
90	Ab initio cluster model approach to the chemisorption of NH3 on Pt(111). Surface Science, 1999, 430, 18-28.	1.9	44

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91	Theoretical Study of NH3 Chemisorption on Pt(111). Computational and Theoretical Chemistry, 1998, 458, 93-98.	1.5	16
92	Absence of collective effects in Heisenberg systems with localized magnetic moments. Physical Review B, 1997, 56, 5069-5072.	3.2	50
93	Ab initio theoretical comparative study of magnetic coupling inKNiF3sandK2NiF4s. Physical Review B, 1997, 55, 4129-4137.	3.2	102
94	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