Mariusz Radon

List of Publications by Year
in descending order

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38 papers	1,461 citations	430874 18 h-index	330143 37 g-index
38 all docs	38 docs citations	38 times ranked	1560 citing authors

#	Article	IF	Citations
1	Structure and mechanistic relevance of Ni2+â€“NO adduct in model HC SCR reaction over NiZSM-5 catalyst â€“ Insights from standard and correlation EPR and IR spectroscopic studies corroborated by molecular modeling. Journal of Catalysis, 2021, 394, 206-219.	6.2	14
2	Spin-state energetics of metallocenes: How do best wave function and density functional theory results compare with the experimental data?. Physical Chemistry Chemical Physics, 2021, 23, 151-172.	2.8	22
3	Zeolites at the Molecular Level: What Can Be Learned from Molecular Modeling. Molecules, 2021, 26, 1511.	3.8	6
4	Experimental and Computational Insight into the Mechanism of NO Binding to Ferric Microperoxidase. The Likely Role of Tautomerization to Account for the pH Dependence. Inorganic Chemistry, 2021, 60, 15948-15967.	4.0	4
5	Heptacoordinated W(IV) Cyanido Supramolecular Complex Trapped by Photolysis of a [W(CN)6(bpy)]2â€“/Zn2+ System. Crystal Growth and Design, 2020, 20, 7742-7749.	3.0	1
6	Benchmarking quantum chemistry methods for spin-state energetics of iron complexes against quantitative experimental data. Physical Chemistry Chemical Physics, 2019, 21, 4854-4870.	2.8	99
7	Toward accurate spin-state energetics of transition metal complexes. Advances in Inorganic Chemistry, 2019, , 221-264.	1.0	10
8	Electronic Properties of Iron Sites and Their Active Forms in Porphyrin-Type Architectures. Springer Series on Bio- and Neurosystems, 2019, , 755-823.	0.2	1
9	Spin States and Other Ligandâ€“Field States of Aqua Complexes Revisited with Multireference ab Initio Calculations Including Solvation Effects. Journal of Chemical Theory and Computation, 2018, 14, 4010-4027.	5.3	26
10	The dependence on ammonia pretreatment of Nâˆ’O activation by Co(II) sites in zeolites: a DFT and ab initio molecular dynamics study. Journal of Molecular Modeling, 2017, 23, 160.	1.8	6
11	Spin-State Energetics of Fe(III) and Ru(III) Aqua Complexes: Accurate ab Initio Calculations and Evidence for Huge Solvation Effects. Journal of Chemical Theory and Computation, 2016, 12, 1592-1605.	5.3	38
12	Mechanism of O₂ Activation by Î±-Ketoglutarate Dependent Oxygenases Revisited. A Quantum Chemical Study. Journal of Physical Chemistry A, 2016, 120, 1261-1274.	2.5	65
13	Ammonia-modified Co(<scp>ii</scp>) sites in zeolites: spin and electron density redistribution through the Co^{II}â€“NO bond. Physical Chemistry Chemical Physics, 2016, 18, 3716-3729.	2.8	16
14	Role of Spin States in Nitric Oxide Binding to Cobalt(II) and Manganese(II) Porphyrins. Is Tighter Binding Always Stronger?. Inorganic Chemistry, 2015, 54, 5634-5645.	4.0	24
15	How can [Mo^{IV}(CN)₆]^{2âˆ’}, an apparently octahedral (d)²complex, be diamagnetic? Insights from quantum chemical calculations and magnetic susceptibility measurements. Physical Chemistry Chemical Physics, 2015, 17, 14890-14902.	2.8	12
16	The effect of Câˆ’HÂ·Â·Â·O bonding and ClÂ·Â·Â·Ï€ interactions in electrocatalytic dehalogenation of C2 chlorides containing an acidic hydrogen. Electrochimica Acta, 2014, 140, 497-504.	5.2	7
17	Mixed-valence VIV/VV tetrametallate core {V4N2O14} cluster containing tris(hydroxymethyl)aminomethane and acetylacetone. Inorganic Chemistry Communication, 2014, 41, 72-75.	3.9	17
18	Nitric oxide as a non-innocent ligand in (bio-)inorganic complexes: Spin and electron transfer in FeIINO bond. Journal of Inorganic Biochemistry, 2014, 136, 147-153.	3.5	13

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19	Mo(IV) and W(IV) cyanido complexes with Schiff bases. Synthesis, X-ray single crystal structures, physicochemical properties and quantum chemical calculations. Polyhedron, 2014, 68, 112-121.	2.2	3
20	Revisiting the role of exact exchange in DFT spin-state energetics of transition metal complexes. Physical Chemistry Chemical Physics, 2014, 16, 14479-14488.	2.8	68
21	Ammonia-modified Co(<scp>ii</scp>) sites in zeolites: IR spectroscopy and spin-resolved charge transfer analysis of NO adsorption complexes. Physical Chemistry Chemical Physics, 2014, 16, 24089-24098.	2.8	4
22	Spin-State Energetics of Heme-Related Models from DFT and Coupled Cluster Calculations. Journal of Chemical Theory and Computation, 2014, 10, 2306-2321.	5.3	93
23	Electronic Properties of Iron Sites and Their Active Forms in Porphyrin-Type Architectures. Springer Series in Bio-/neuroinformatics, 2014, , 711-782.	0.1	0
24	On the role of noncovalent interactions in electrocatalysis. Two cases of mediated reductive dehalogenation. Electrochimica Acta, 2013, 110, 619-627.	5.2	9
25	Electronic propensity of Cu(II) versus Cu(I) sites in zeolites to activate NO â€" Spin- and orbital-resolved Cuâ€"NO electron transfer. Canadian Journal of Chemistry, 2013, 91, 538-543.	1.1	9
26	Autocatalytic cathodic dehalogenation triggered by dissociative electron transfer through a Câ€"Hâ‹¯O hydrogen bond. Physical Chemistry Chemical Physics, 2013, 15, 17522.	2.8	9
27	On the nature of spin- and orbital-resolved Cu+â€"NO charge transfer in the gas phase and at Cu(I) sites in zeolites. Structural Chemistry, 2012, 23, 1349-1356.	2.0	15
28	DFT and Ab Initio Study of Iron-Oxo Porphyrins: May They Have a Low-Lying Iron(V)-Oxo Electromer?. Journal of Chemical Theory and Computation, 2011, 7, 898-908.	5.3	71
29	Mono- and Dinitrosyls on Copper(I) Site in a Zeolite Model: Effects of Static Correlation. Journal of Physical Chemistry A, 2011, 115, 11761-11774.	2.5	12
30	Spin Ground State and Magnetic Properties of Cobalt(II): Relativistic DFT Calculations Guided by EPR Measurements of Bis(2,4-acetylacetonate)cobalt(II)-Based Complexes. Journal of Physical Chemistry A, 2011, 115, 2316-2324.	2.5	36
31	Electronic Structure of Selected {FeNO}⁷ Complexes in Heme and Non-Heme Architectures: A Density Functional and Multireference ab Initio Study. Journal of Physical Chemistry B, 2010, 114, 1518-1528.	2.6	147
32	Mechanism of Selective Halogenation by SyrB2: A Computational Study. Journal of the American Chemical Society, 2010, 132, 12887-12898.	13.7	98
33	Performance of CASPT2 and DFT for Relative Spin-State Energetics of Heme Models. Journal of Chemical Theory and Computation, 2010, 6, 576-582.	5.3	147
34	Conformational Stability and Spin States of Cobalt(II) Acetylacetonate: CASPT2 and DFT Study. Journal of Chemical Theory and Computation, 2009, 5, 1237-1244.	5.3	30
35	On the properties of natural orbitals for chemical valence. Theoretical Chemistry Accounts, 2008, 120, 337-339.	1.4	45
36	Nitrogen Monoxide Interaction with Cu(I) Sites in Zeolites X and Y: Quantum Chemical Calculations and IR Studies. Journal of Physical Chemistry C, 2008, 112, 17998-18010.	3.1	30

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37	Binding of CO, NO, and O₂ to Heme by Density Functional and Multireference ab Initio Calculations. Journal of Physical Chemistry A, 2008, 112, 11824-11832.	2.5	218
38	Peculiarities of the Electronic Structure of Cytochrome P450 Compound I:â€‰ CASPT2 and DFT Modeling. Journal of Chemical Theory and Computation, 2007, 3, 728-734.	5.3	36