Russo Nino

List of Publications by Year
in descending order

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438	15,433	20797 60	34964 98
papers	citations	h-index	g-index

446	446	446	12612
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The molecular basis of working mechanism of natural polyphenolic antioxidants. Food Chemistry, 2011, 125, 288-306.	4.2	917
2	Antioxidant Properties of Phenolic Compounds:Â H-Atom versus Electron Transfer Mechanism. Journal of Physical Chemistry A, 2004, 108, 4916-4922.	1.1	553
3	Iron Chelation by the Powerful Antioxidant Flavonoid Quercetin. Journal of Agricultural and Food Chemistry, 2006, 54, 6343-6351.	2.4	387
4	Food Antioxidants: Chemical Insights at the Molecular Level. Annual Review of Food Science and Technology, 2016, 7, 335-352.	5.1	294
5	Structure, Conformation, and Electronic Properties of Apigenin, Luteolin, and Taxifolin Antioxidants. A First Principle Theoretical Study. Journal of Physical Chemistry A, 2004, 108, 92-96.	1.1	280
6	LANL2DZ basis sets recontracted in the framework of density functional theory. Journal of Chemical Physics, 2006, 125, 104107.	1.2	227
7	Antioxidant Activity of trans-Resveratrol toward Hydroxyl and Hydroperoxyl Radicals: A Quantum Chemical and Computational Kinetics Study. Journal of Organic Chemistry, 2012, 77, 3868-3877.	1.7	226
8	A physicochemical examination of the free radical scavenging activity of Trolox: mechanism, kinetics and influence of the environment. Physical Chemistry Chemical Physics, 2013, 15, 4642.	1.3	210
9	Density functional computations of the energetic and spectroscopic parameters of quercetin and its radicals in the gas phase and in solvent. Theoretical Chemistry Accounts, 2004, 111, 210-216.	0.5	159
10	Bond Energies and Attachments Sites of Sodium and Potassium Cations to DNA and RNA Nucleic Acid Bases in the Gas Phase. Journal of the American Chemical Society, 2001, 123, 10272-10279.	6.6	154
11	A density functional study of small copper clusters: Cun (nâ©½5). Journal of Chemical Physics, 1996, 105, 9546-9556.	1.2	153
12	Theoretical determination of electron affinity and ionization potential of DNA and RNA bases. Journal of Computational Chemistry, 2000, 21, 1243-1250.	1.5	141
13	Radical Scavenging Ability of Gallic Acid toward OH and OOH Radicals. Reaction Mechanism and Rate Constants from the Density Functional Theory. Journal of Physical Chemistry B, 2014, 118, 10380-10389.	1.2	139
14	Semiempirical Molecular Modeling into Quercetin Reactive Site:Â Structural, Conformational, and Electronic Features. Journal of Agricultural and Food Chemistry, 2000, 48, 3232-3237.	2.4	128
15	Protonation of thymine, cytosine, adenine, and guanine DNA nucleic acid bases: Theoretical investigation into the framework of density functional theory. Journal of Computational Chemistry, 1998, 19, 989-1000.	1.5	127
16	Interaction of cysteine with Cu2+ and group IIb (Zn2+, Cd2+, Hg2+) metal cations: a theoretical study. Journal of Mass Spectrometry, 2005, 40, 300-306.	0.7	121
17	Gas-phase metal ion (Li+, Na+, Cu+) affinities of glycine and alanine. Journal of Inorganic Biochemistry, 2000, 79, 179-185.	1.5	114
18	Theoretical Study of Two-State Reactivity of Transition Metal Cations:Â The â€œDifficultâ€•Case of Iron Ion Interacting with Water, Ammonia, and Methane. Journal of Physical Chemistry A, 2004, 108, 1069-1081.	1.1	112

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19	On the Hydrolysis Mechanism of the Secondâ€Generation Anticancer Drug Carboplatin. Chemistry - A European Journal, 2007, 13, 10108-10116.	1.7	111
20	Gas and Liquid Phase Acidity of Natural Antioxidants. Journal of Agricultural and Food Chemistry, 2006, 54, 3078-3085.	2.4	108
21	Structural and Electronic Characterization of the Complexes Obtained by the Interaction between Bare and Hydrated First-Row Transition-Metal Ions (Mn2+, Fe2+, Co2+, Ni2+, Cu2+, Zn2+) and Glycine. Journal of Physical Chemistry B, 2006, 110, 24666-24673.	1.2	106
22	Spectroscopic Properties of Porphyrin-Like Photosensitizers:Â Insights from Theory. Journal of Physical Chemistry B, 2006, 110, 2398-2404.	1.2	106
23	Lithium Affinity for DNA and RNA Nucleobases. The Role of Theoretical Information in the Elucidation of the Mass Spectrometry Data. Journal of Physical Chemistry B, 2001, 105, 4735-4741.	1.2	105
24	About the Mulliken electronegativity in DFT. Theoretical Chemistry Accounts, 2005, 114, 38-45.	0.5	104
25	Interaction of Li+, Na+, and K+ with the Proline Amino Acid. Complexation Modes, Potential Energy Profiles, and Metal Ion Affinities. Journal of Physical Chemistry B, 2003, 107, 2588-2594.	1.2	103
26	Pyranoanthocyanins: A Theoretical Investigation on Their Antioxidant Activity. Journal of Agricultural and Food Chemistry, 2010, 58, 8862-8871.	2.4	101
27	Detailed Investigation of the OH Radical Quenching by Natural Antioxidant Caffeic Acid Studied by Quantum Mechanical Models. Journal of Chemical Theory and Computation, 2011, 7, 4218-4233.	2.3	100
28	Density-Functional Approach to Hardness Evaluation and Its Use in the Study of the Maximum Hardness Principle. Journal of the American Chemical Society, 1998, 120, 9053-9058.	6.6	99
29	The Second-Generation Anticancer Drug Nedaplatin: A Theoretical Investigation on the Hydrolysis Mechanism. Journal of Physical Chemistry B, 2009, 113, 14473-14479.	1.2	98
30	Reaction of Sc+(1D,3D) with H2O, NH3, and CH4:Â A Density Functional Study. Journal of the American Chemical Society, 2001, 123, 2588-2596.	6.6	97
31	Structures and Electronic Absorption Spectra of a Recently Synthesised Class of Photodynamic Therapy Agents. Chemistry - A European Journal, 2006, 12, 6797-6803.	1.7	95
32	Theoretical Study of Ammonia and Methane Activation by First-Row Transition Metal Cations M+(M =) Tj ETQq0 0 0 rgBT /Overlock 10 T	6.6	93
33	OsB2 and RuB2, ultra-incompressible, hard materials: First-principles electronic structure calculations. Chemical Physics Letters, 2006, 425, 311-314.	1.2	93
34	The inactivation of lipid peroxide radical by quercetin. A theoretical insight. Physical Chemistry Chemical Physics, 2010, 12, 7662.	1.3	92
35	A combined theoretical and experimental study on the oxidation of fulvic acid by the sulfate radical anion. Photochemical and Photobiological Sciences, 2009, 8, 992-997.	1.6	85
36	A molecular simulation study on gas diffusion in a dense poly(etherâ€“etherâ€“ketone) membrane. Polymer, 2001, 42, 521-533.	1.8	83

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37	Theoretical and Experimental Investigation on the Oxidation of Gallic Acid by Sulfate Radical Anions. Journal of Physical Chemistry A, 2008, 112, 1188-1194.	1.1	82
38	Proton Affinity and Protonation Sites of Aniline. Energetic Behavior and Density Functional Reactivity Indices. Journal of Physical Chemistry A, 2000, 104, 4017-4021.	1.1	79
39	Antioxidant properties of several coumarinâ€“chalcone hybrids from theoretical insights. RSC Advances, 2015, 5, 565-575.	1.7	79
40	Neutral and Acidic Hydrolysis Reactions of the Third Generation Anticancer Drug Oxaliplatin. Journal of Physical Chemistry B, 2009, 113, 831-838.	1.2	77
41	Absorption Spectra of First-Row Transition Metal Complexes of Bacteriochlorins:â€‰ A Theoretical Analysis. Journal of Physical Chemistry B, 2005, 109, 12214-12221.	1.2	76
42	Spinâ€“Orbit Charge Recombination Intersystem Crossing in Phenothiazineâ€“Anthracene Compact Dyads: Effect of Molecular Conformation on Electronic Coupling, Electronic Transitions, and Electron Spin Polarizations of the Triplet States. Journal of Physical Chemistry C, 2018, 122, 27850-27865.	1.5	76
43	Spinâ€“Orbit Chargeâ€Transfer Intersystem Crossing (ISC) in Compact Electron Donorâ€“Acceptor Dyads: ISC Mechanism and Application as Novel and Potent Photodynamic Therapy Reagents. Chemistry - A European Journal, 2020, 26, 1091-1102.	1.7	76
44	A Comparative Study of the Catalytic Mechanisms of the Zinc and Cadmium Containing Carbonic Anhydrase. Journal of the American Chemical Society, 2005, 127, 4242-4253.	6.6	75
45	Fukui Indices from Perturbed Kohnâ^'Sham Orbitals and Regional Softness from Mayer Atomic Valences. Journal of Physical Chemistry A, 2001, 105, 1959-1967.	1.1	74
46	Gas-Phase Chemistry of Actinides Ions:Â New Insights into the Reaction of UO+and UO2+with Water. Journal of the American Chemical Society, 2007, 129, 4229-4239.	6.6	74
47	Enzymatic Flexibility and Reaction Rate: A QM/MM Study of HIV-1 Protease. ACS Catalysis, 2015, 5, 5617-5626.	5.5	72
48	On the Hardness Evaluation in Solvent for Neutral and Charged Systems. Journal of the American Chemical Society, 2002, 124, 1494-1499.	6.6	70
49	Mechanism of Nitrate Reduction byDesulfovibrio desulfuricans Nitrate Reductaseâ€”A Theoretical Investigation. Chemistry - A European Journal, 2006, 12, 2532-2541.	1.7	70
50	Peptide Hydrolysis by the Binuclear Zinc Enzyme Aminopeptidase from Aeromonas proteolytica:â€‰ A Density Functional Theory Study. Journal of Physical Chemistry B, 2008, 112, 2494-2500.	1.2	68
51	Understanding Zinc(II) Chelation with Quercetin and Luteolin: A Combined NMR and Theoretical Study. Journal of Physical Chemistry B, 2015, 119, 83-95.	1.2	68
52	Gas-Phase Absolute Ca2+and Mg2+Affinity for Nucleic Acid Bases. A Theoretical Determination. Journal of Physical Chemistry A, 2003, 107, 11533-11538.	1.1	67
53	Breaking the barrier: an osmium photosensitizer with unprecedented hypoxic phototoxicity for real world photodynamic therapy. Chemical Science, 2020, 11, 9784-9806.	3.7	67
54	Potential Energy Surfaces for the Gas-Phase Interaction between Î±-Alanine and Alkali Metal Ions (Li+,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.9	66

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55	Topological Analysis of the Reaction of Mn+(7S,5S) with H2O, NH3, and CH4Molecules. Journal of Physical Chemistry A, 2003, 107, 4862-4868.	1.1	65
56	Atomic Radii Scale and Related Size Properties from Density Functional Electronegativity Formulation. Journal of Physical Chemistry A, 2003, 107, 5461-5465.	1.1	65
57	Structural and Electronic Characterization of Antioxidants from Marine Organisms. Theoretical Chemistry Accounts, 2006, 115, 361-369.	0.5	65
58	Spectrophotometric study of the copigmentation of malvidin 3-O-glucoside with p-coumaric, vanillic and syringic acids. Food Chemistry, 2013, 141, 3614-3620.	4.2	65
59	On the Inhibitor Effects of Bergamot Juice Flavonoids Binding to the 3-Hydroxy-3-methylglutaryl-CoA Reductase (HMGR) Enzyme. Journal of Agricultural and Food Chemistry, 2010, 58, 10768-10773.	2.4	64
60	A Computational Study (TDDFT and RICC2) of the Electronic Spectra of Pyranoanthocyanins in the Gas Phase and Solution. Journal of Chemical Theory and Computation, 2011, 7, 1073-1081.	2.3	62
61	Newly developed basis sets for density functional calculations. Journal of Computational Chemistry, 2005, 26, 175-184.	1.5	58
62	Which One among Zn(II), Co(II), Mn(II), and Fe(II) is the Most Efficient Ion for the Methionine Aminopeptidase Catalyzed Reaction?. Journal of the American Chemical Society, 2007, 129, 7776-7784.	6.6	57
63	Density functional study of the antioxidant activity of some recently synthesized resveratrol analogues. Food Chemistry, 2013, 141, 2017-2024.	4.2	57
64	The heavy atom effect on Zn(<scp>ii</scp>) phthalocyanine derivatives: a theoretical exploration of the photophysical properties. Physical Chemistry Chemical Physics, 2015, 17, 23595-23601.	1.3	57
65	Theoretical Exploration of Type I/Type II Dual Photoreactivity of Promising Ru(II) Dyads for PDT Approach. Inorganic Chemistry, 2016, 55, 11185-11192.	1.9	57
66	Density functional approach to the structures and EPR parameters of open shell systems. The case of fluorovinyl radicals. Chemical Physics Letters, 1993, 212, 5-11.	1.2	56
67	On the applicability of the HSAB principle through the use of improved computational schemes for chemical hardness evaluation. Journal of Computational Chemistry, 2004, 25, 994-1003.	1.5	56
68	Human Insulin-Degrading Enzyme Working Mechanism. Journal of the American Chemical Society, 2009, 131, 14804-14811.	6.6	56
69	Theoretical Determination of Electronic Spectra and Intersystem Spinâ€“Orbit Coupling: The Case of Isoindole-BODIPY Dyes. Journal of Chemical Theory and Computation, 2014, 10, 4006-4013.	2.3	55
70	Which One among the Pt-Containing Anticancer Drugs More Easily Forms Monoadducts with G and A DNA Bases? A Comparative Study among Oxaliplatin, Nedaplatin, and Carboplatin. Inorganic Chemistry, 2011, 50, 6965-6971.	1.9	54
71	Catalytic activity of a Î¶-class zinc and cadmium containing carbonic anhydrase. Compared work mechanisms. Physical Chemistry Chemical Physics, 2011, 13, 3468.	1.3	54
72	General trends in the molecular physics of azabiphenyls. Molecular Physics, 1983, 49, 599-619.	0.8	53

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73	V3: Structure and vibrations from density functional theory, Franckâ€“Condon factors, and the pulsed-field ionization zero-electron-kinetic energy spectrum. Journal of Chemical Physics, 2001, 114, 4036-4044.	1.2	53
74	Gas-phase theoretical prediction of the metal affinity of copper(I) ion for DNA and RNA bases. Journal of Mass Spectrometry, 2003, 38, 265-270.	0.7	53
75	Halogen atom effect on the photophysical properties of substituted aza-BODIPY derivatives. Physical Chemistry Chemical Physics, 2017, 19, 2530-2536.	1.3	53
76	Catalytic Mechanism of the Arylsulfatase Promiscuous Enzyme from Pseudomonas Aeruginosa. Chemistry - A European Journal, 2013, 19, 2185-2192.	1.7	52
77	First-Principle Time-Dependent Study of Magnesium-Containing Porphyrin-Like Compounds Potentially Useful for Their Application in Photodynamic Therapy. Journal of Physical Chemistry B, 2008, 112, 4123-4130.	1.2	49
78	Gas-Phase Reactions of the Bare Th²⁺ and U²⁺ Ions with Small Alkanes, CH₄, C₂H₆, and C₃H₈: Experimental and Theoretical Study of Elementary Organoactinide Chemistry. Journal of the American Chemical Society, 2011, 133, 1955-1970.	6.6	49
79	The Preferred Reaction Path for the Oxidation of Methanol by PQQ-Containing Methanol Dehydrogenase: Additionâ€“Elimination versus Hydride-Transfer Mechanism. Chemistry - A European Journal, 2007, 13, 2109-2117.	1.7	48
80	Antioxidant properties comparative study of natural hydroxycinnamic acids and structurally modified derivatives: Computational insights. Computational and Theoretical Chemistry, 2016, 1077, 39-47.	1.1	48
81	A Comparative Study of the Antioxidant Power of Flavonoid Catechin and Its Planar Analogue. Journal of Agricultural and Food Chemistry, 2007, 55, 7944-7949.	2.4	47
82	Reaction Mechanism of Molybdoenzyme Formate Dehydrogenase. Chemistry - A European Journal, 2008, 14, 8674-8681.	1.7	47
83	Methane Câˆ’H Bond Activation by Gas-Phase Th⁺and U⁺: Reaction Mechanisms and Bonding Analysis. Organometallics, 2009, 28, 3716-3726.	1.1	47
84	Photophysical origin of the reduced photodynamic therapy activity of temocene compared to FoscanÂ®: insights from theory. Physical Chemistry Chemical Physics, 2013, 15, 16167.	1.3	47
85	Topological Analysis of the Reaction of Uranium Ions (U⁺, U²⁺) with N₂O in the Gas Phase. Journal of Physical Chemistry A, 2008, 112, 12966-12974.	1.1	45
86	Investigation of the host-guest complexation between 4-sulfocalix[4]arene and nedaplatin for potential use in drug delivery. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 193, 528-536.	2.0	45
87	Insertion Reaction of Mn+Bare Metal Cation into the Nâˆ’H and Câˆ’H Bonds of Ammonia and Methane. Journal of Physical Chemistry A, 2002, 106, 8937-8944.	1.1	44
88	On the Potential Use of Squaraine Derivatives as Photosensitizers in Photodynamic Therapy: A TDDFT and RICC2 Survey. Journal of Chemical Theory and Computation, 2009, 5, 1849-1857.	2.3	44
89	Density Functional Predictions of Antioxidant Activity and UV Spectral Features of Nasutin A, Isonasutin, Ellagic Acid, and One of Its Possible Derivatives. Journal of Agricultural and Food Chemistry, 2013, 61, 9650-9657.	2.4	44
90	The Catalytic Mechanism of Protein Phosphataseâ€…5 Established by DFT Calculations. Chemistry - A European Journal, 2013, 19, 14081-14089.	1.7	44

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91	Metal Atom Effect on the Photophysical Properties of Mg(II), Zn(II), Cd(II), and Pd(II) Tetraphenylporphyrin Complexes Proposed as Possible Drugs in Photodynamic Therapy. Molecules, 2017, 22, 1093.	1.7	44
92	The role of glutathione in cadmium ion detoxification: Coordination modes and binding properties â€“ A density functional study. Journal of Inorganic Biochemistry, 2009, 103, 50-57.	1.5	43
93	Correlation between Energy, Polarizability, and Hardness Profiles in the Isomerization Reaction of HNO and ClNO. Journal of Physical Chemistry A, 2001, 105, 442-450.	1.1	42
94	Photophysical properties of free and metallated meso-substituted tetrabenzotriazaporphyrin from density functional theory investigation. Dyes and Pigments, 2015, 120, 335-339.	2.0	42
95	Protonation of glycine and alanine: proton affinities, intrinsic basicities and proton transfer path. Computational and Theoretical Chemistry, 1998, 430, 41-49.	1.5	41
96	Gas-phase interaction between DNA and RNA bases and copper (II) ion: A density functional study. International Journal of Quantum Chemistry, 2004, 98, 347-354.	1.0	41
97	PDT-correlated photophysical properties of thienopyrrole BODIPY derivatives. Theoretical insights. Dyes and Pigments, 2016, 130, 9-15.	2.0	41
98	Coumarinâ€“Chalcone Hybrids as Peroxyl Radical Scavengers: Kinetics and Mechanisms. Journal of Chemical Information and Modeling, 2016, 56, 662-670.	2.5	41
99	Model potential for As and LCGTO MP LSD calculation of geometry, electronic structure and photoelectron spectra for As2 and As4. Chemical Physics Letters, 1987, 142, 169-174.	1.2	40
100	How Can Uranium Ions (U+, U2+) Activate the Oï£¿H Bond of Water in the Gas Phase?. Angewandte Chemie - International Edition, 2006, 45, 1095-1099.	7.2	40
101	The Degradation Pathways in Chloride Medium of the Third Generation Anticancer Drug Oxaliplatin. Journal of Physical Chemistry B, 2008, 112, 10765-10768.	1.2	40
102	Homogeneous Gold Catalysis: Hydration of 1,2-Diphenylacetylene with Methanol in Aqueous Media. A Theoretical Viewpoint. Organometallics, 2012, 31, 3074-3080.	1.1	40
103	Photophysical properties prediction of selenium- and tellurium-substituted thymidine as potential UVA chemotherapeutic agents. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	40
104	Ab-initio mechanistic studies of radical reactions. Directive effects in the addition of methyl radical to unsymmetrical fluoroethenes. Journal of the Chemical Society Perkin Transactions II, 1986, , 1517-1524.	0.9	39
105	On the Pt⁺ and Rh⁺ Catalytic Activity in the Nitrous Oxide Reduction by Carbon Monoxide. Journal of Chemical Theory and Computation, 2008, 4, 1886-1890.	2.3	39
106	Theoretical Study of Silver-Ion-Mediated Base Pairs: The Case of Câ€“Agâ€“C and Câ€“Agâ€“A Systems. Journal of Physical Chemistry A, 2015, 119, 5153-5157.	1.1	39
107	B,Nâ€Codoped graphene as catalyst for the oxygen reduction reaction: Insights from periodic and cluster DFT calculations. Journal of Computational Chemistry, 2018, 39, 637-647.	1.5	39
108	Interaction of Cu+ and Cu2+ ions with ?-alanine. A density functional study. Journal of Mass Spectrometry, 2002, 37, 786-791.	0.7	38

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109	Absorption Spectra of the Potential Photodynamic Therapy Photosensitizers Texaphyrins Complexes:â€‰ A Theoretical Analysis. Journal of Chemical Theory and Computation, 2007, 3, 860-869.	2.3	38
110	Hydration of ionic species studied by the reference interaction site model with a repulsive bridge correction. Journal of Computational Chemistry, 2008, 29, 2406-2415.	1.5	38
111	A Proposal for Mitochondrial Processing Peptidase Catalytic Mechanism. Journal of the American Chemical Society, 2011, 133, 17824-17831.	6.6	38
112	Complexation behaviour of caffeic, ferulic and p-coumaric acids towards aluminium cations: a combined experimental and theoretical approach. New Journal of Chemistry, 2017, 41, 5182-5190.	1.4	38
113	How Can Methanol Dehydrogenase from Methylacidiphilum fumariolicum Work with the Alien Ce^{III} Ion in the Active Center? Aâ€…Theoretical Study. Chemistry - A European Journal, 2017, 23, 8652-8657.	1.7	38
114	Experimental and Theoretical Investigation on the Catalytic Generation of Environmentally Persistent Free Radicals from Benzene. Journal of Physical Chemistry C, 2017, 121, 9381-9393.	1.5	38
115	Density Functional Study of Ammonia Activation by Late First-Row Transition Metal Cations. Inorganic Chemistry, 2004, 43, 4944-4952.	1.9	37
116	The role of quantum chemistry in the elucidation of the elementary mechanisms of catalytic processes: from atoms, to surfaces, to enzymes. Theoretical Chemistry Accounts, 2007, 117, 765-779.	0.5	37
117	The mutual influence of non-covalent interactions in Ï€-electron deficient cavities: the case of anion recognition by tetraoxacalix[2]arene[2]triazine. Chemical Communications, 2010, 46, 5894.	2.2	37
118	Can Human Prolidase Enzyme Use Different Metals for Full Catalytic Activity?. Inorganic Chemistry, 2011, 50, 3394-3403.	1.9	37
119	Evidence for the Formation of a Moâ€“H Intermediate in the Catalytic Cycle of Formate Dehydrogenase. Inorganic Chemistry, 2012, 51, 8331-8339.	1.9	37
120	Can Expanded Bacteriochlorins Act as Photosensitizers in Photodynamic Therapy? Good News from Density Functional Theory Computations. Molecules, 2016, 21, 288.	1.7	37
121	Os(II) Oligothienyl Complexes as a Hypoxia-Active Photosensitizer Class for Photodynamic Therapy. Inorganic Chemistry, 2020, 59, 16341-16360.	1.9	37
122	Acetylene Cyclotrimerization by Early Second-Row Transition Metals in the Gas Phase. A Theoretical Study. Inorganic Chemistry, 2005, 44, 9807-9816.	1.9	36
123	Interaction of CO with PdAu(111) and PdAu(100) Bimetallic Surfaces:â€‰ A Theoretical Cluster Model Study. Journal of Physical Chemistry C, 2008, 112, 6073-6081.	1.5	36
124	Atomistic details of the Catalytic Mechanism of Fe(III)â^'Zn(II) Purple Acid Phosphatase. Journal of Chemical Theory and Computation, 2010, 6, 2424-2433.	2.3	36
125	Hydration of gas-phase ytterbium ion complexes studied by experiment and theory. Theoretical Chemistry Accounts, 2011, 129, 575-592.	0.5	36
126	The performance of density functional based methods in the description of selected biological systems and processes. Physical Chemistry Chemical Physics, 2012, 14, 14943.	1.3	36

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127	Theoretical calculations of glycine and alanine gas-phase acidities. Journal of the American Society for Mass Spectrometry, 1999, 10, 318-322.	1.2	35
128	Mechanistic Aspects of the Reaction of Th⁺ and Th²⁺ with Water in the Gas Phase. Inorganic Chemistry, 2008, 47, 2083-2088.	1.9	35
129	Rhenium(iv) compounds inducing apoptosis in cancer cells. Chemical Communications, 2011, 47, 5283.	2.2	35
130	Insights into the coordination mode of quercetin with the Al(<scp>iii</scp>) ion from a combined experimental and theoretical study. Dalton Transactions, 2014, 43, 7269-7274.	1.6	35
131	Oxidation of Ethylbenzene to Acetophenone with N-Doped Graphene: Insight from Theory. Journal of Physical Chemistry C, 2014, 118, 12275-12284.	1.5	35
132	Investigation of the Inertness to Hydrolysis of Platinum(IV) Prodrugs. Inorganic Chemistry, 2016, 55, 1580-1586.	1.9	35
133	Photophysical Properties of S, Se and Te-Substituted Deoxyguanosines: Insight into Their Ability To Act as Chemotherapeutic Agents. Journal of Chemical Information and Modeling, 2017, 57, 234-242.	2.5	35
134	Conformational behaviour of isomeric bithienyls. An ab initio study. Journal of the Chemical Society Perkin Transactions II, 1986, , 907.	0.9	34
135	On the Copper(II) Ion Coordination by Prion Protein HGGGW Pentapeptide Model. Journal of Physical Chemistry B, 2007, 111, 635-640.	1.2	34
136	DFT spinâ€“orbit coupling between singlet and triplet excited states: A case of psoralen compounds. Chemical Physics Letters, 2010, 490, 90-96.	1.2	34
137	Mechanistic Investigation of the Hydrogenation of O2 by a Transfer Hydrogenation Catalyst. Journal of the American Chemical Society, 2010, 132, 4178-4190.	6.6	34
138	Synergistic Effects of Metals in a Promising Ru^{II}â”Pt^{II} Assembly for a Combined Anticancer Approach: Theoretical Exploration of the Photophysical Properties. Chemistry - A European Journal, 2016, 22, 9162-9168.	1.7	34
139	The Effects of the Metal Ion Substitution into the Active Site of Metalloenzymes: A Theoretical Insight on Some Selected Cases. Catalysts, 2020, 10, 1038.	1.6	34
140	Experimental and theoretical approach to the electronic structure and the molecular conformation of azabiphenyls. Assymetric bipyridines. Chemical Physics, 1985, 96, 435-445.	0.9	33
141	On the interaction between manganese cation (Mn2+) and the nucleic acid bases (T, U, C, A, G) in the gas phase. International Journal of Quantum Chemistry, 2002, 90, 903-909.	1.0	33
142	A quasilinear RISM approach for the computation of solvation free energy of ionic species. Chemical Physics Letters, 2006, 418, 485-489.	1.2	33
143	Methane activation by chromium oxide cations in the gas phase: A theoretical study. Journal of Computational Chemistry, 2006, 27, 174-187.	1.5	33
144	On the Origin of the Different Performance of Iron and Manganese Monocations in Catalyzing the Nitrous Oxide Reduction by Carbon Oxide. Inorganic Chemistry, 2007, 46, 7489-7493.	1.9	33

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145	Experimental and theoretical characterization of a new synthesized extended viologen. Chemical Physics Letters, 2012, 552, 141-145.	1.2	33
146	Bisanthracene Bis(dicarboxylic imide)s as Potential Photosensitizers in Photodynamic Therapy: A Theoretical Investigation. Journal of Chemical Information and Modeling, 2013, 53, 2334-2340.	2.5	33
147	Photophysical properties of NIR-emitting fluorescence probes: insights from TD-DFT. Physical Chemistry Chemical Physics, 2013, 15, 10019.	1.3	33
148	Role of the Metal Ion in Formylâ˜Peptide Bond Hydrolysis by a Peptide Deformylase Active Site Model. Journal of Physical Chemistry B, 2006, 110, 1063-1072.	1.2	32
149	Establishing the Catalytic Mechanism of Human Pancreatic Î±-Amylase with QM/MM Methods. Journal of Chemical Theory and Computation, 2015, 11, 2508-2516.	2.3	32
150	Insight on the chelation of aluminum(III) and iron(III) by curcumin in aqueous solution. Journal of Molecular Liquids, 2019, 296, 111805.	2.3	32
151	Chemisorption of atomic and molecular oxygen on the (100) surface of silicon; a theoretical study. Surface Science, 1985, 162, 230-238.	0.8	31
152	Diffusion of gases in PEEKs membranes: molecular dynamics simulations. Journal of Membrane Science, 2002, 206, 389-398.	4.1	31
153	On the metal ion (Zn2+, Cu2+) coordination with beta-amyloid peptide: DFT computational study. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 57-69.	2.2	31
154	Electronic spectra and intersystem spinâ€orbit coupling in 1,2â€and 1,3â€squaraines. Journal of Computational Chemistry, 2014, 35, 2107-2113.	1.5	31
155	On the chemisorption of water on the (100) surface of silicon. Surface Science, 1987, 180, 599-604.	0.8	30
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