Mansour Zahedi

List of Publications by Year
in descending order

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130	1,376	394390	434170
papers	citations	19 h-index	31 g-index

133	133	133	1428
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A DFT comparative study of single and double SO2 adsorption on Pt-doped and Au-doped single-walled carbon nanotube. Applied Surface Science, 2015, 349, 864-869.	6.1	91
2	266 nm CH3I photodissociation: CH3 spectra and population distributions by coherent Raman spectroscopy. Journal of Chemical Physics, 1994, 100, 4043-4055.	3.0	63
3	Rate constants for CN reactions with hydrocarbons and the product HCN vibrational populations: Examples of heavyâ€“lightâ€“heavy abstraction reactions. Journal of Chemical Physics, 1992, 96, 5817-5826.	3.0	59
4	High resolution study of the Î½1 vibration of CH3 by coherent Raman photofragment spectroscopy. Journal of Chemical Physics, 1992, 96, 1822-1831.	3.0	58
5	Rheo-Optical Fourier Transform Infrared and Raman Spectroscopy of Polymers. Applied Spectroscopy, 1993, 47, 1531-1539.	2.2	55
6	To What Extent are â€œAtoms in Moleculesâ€•Structures of Hydrocarbons Reproducible from the Promolecule Electron Densities?. Chemistry - A European Journal, 2016, 22, 5003-5009.	3.3	48
7	Unique 1âˆ¶2 adduct formation of meso-tetraarylporphyrins and meso-tetraalkylporphyrins with BF3: a spectroscopic and ab initio study. New Journal of Chemistry, 2004, 28, 1600-1607.	2.8	46
8	A Theoretical Elucidation of Glucose Interaction with HSA's Domains. Journal of Biomolecular Structure and Dynamics, 2010, 28, 211-226.	3.5	41
9	DFT/B3LYP study of the substituent effect on the reaction enthalpies of the individual steps of single electron transferâ€“proton transfer and sequential proton loss electron transfer mechanisms of chroman derivatives antioxidant action. Computational and Theoretical Chemistry, 2011, 969, 1-12.	2.5	36
10	Density Functional Theory (B3LYP) Study of Substituent Effects on Oâ€“H Bond Dissociation Enthalpies of trans-Resveratrol Derivatives and the Role of Intramolecular Hydrogen Bonds. Journal of Organic Chemistry, 2012, 77, 10093-10104.	3.2	36
11	Polyacenes electronic properties and their dependence on molecular size. Computational and Theoretical Chemistry, 2008, 862, 7-15.	1.5	29
12	DFT/B3LYP study of the solvent effect on the reaction enthalpies of homolytic and heterolytic OH bond cleavage in mono-substituted chromans. Computational and Theoretical Chemistry, 2011, 978, 16-28.	2.5	29
13	DFT/B3LYP study of the substituent effects on OH bond dissociation enthalpies of chroman derivatives in the gas phase and solvent environment. Computational and Theoretical Chemistry, 2011, 965, 114-122.	2.5	29
14	Kinetics and Mechanism of the Autocatalytic Oxidation of L-Asparagine in a Moderately Concentrated Sulfuric Acid Medium. Kinetics and Catalysis, 2004, 45, 351-358.	1.0	27
15	Non-adiabatic interactions in excitedC 2 H molecules and their relationship toC 2 formation in comets. Astrophysics and Space Science, 1996, 236, 29-47.	1.4	22
16	The Role of Observables and Non-observables in Chemistry: A Critique of Chemical Language. Foundations of Chemistry, 2006, 8, 37-52.	1.1	22
17	Quantum chemical investigation of intramolecular thione-thiol tautomerism of 1,2,4-triazole-3-thione and its disubstituted derivatives. Journal of Molecular Modeling, 2010, 16, 841-855.	1.8	22
18	Use of seeded Nd:YAG lasers for high-resolution spectroscopy. Optics Letters, 1993, 18, 149.	3.3	20

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19	Cross-Linking Mechanisms of Arginine and Lysine with Î±,Î²-Dicarbonyl Compounds in Aqueous Solution. Journal of Physical Chemistry A, 2011, 115, 13542-13555.	2.5	19
20	Theoretical investigations of the hydrolysis pathway of verdoheme to biliverdin. Journal of Inorganic Biochemistry, 2007, 101, 385-395.	3.5	18
21	Effect of Axial Ligand on the Electronic Configuration, Spin States, and Reactivity of Iron Oxophlorin. Inorganic Chemistry, 2012, 51, 7094-7102.	4.0	17
22	Fullerene-C 60 and crown ether doped on C 60 sensors for high sensitive detection of alkali and alkaline earth cations. Physica E: Low-Dimensional Systems and Nanostructures, 2017, 87, 51-58.	2.7	17
23	Carbonic anhydrase inhibitors: A quantum mechanical study of interaction between some antiepileptic drugs with active center of carbonic anhydrase enzyme. Computational and Theoretical Chemistry, 2012, 992, 59-69.	2.5	16
24	Protective effect of rutin (vitamin p) against heme oxidation: A quantum mechanical approach. Computational and Theoretical Chemistry, 2012, 996, 28-36.	2.5	16
25	Theoretical investigations of the reactivity of verdoheme analogues: Opening of the planar macrocycle by amide, dimethyl amide, and hydroxide nucleophiles to form helical biliverdin type complexes. Journal of Inorganic Biochemistry, 2006, 100, 1449-1461.	3.5	15
26	Delayed autocatalytic behavior of Mn(II) ions at a critical ratio: The effect of structural isomerism on permanganic oxidation ofL-norleucine. International Journal of Chemical Kinetics, 2006, 38, 1-11.	1.6	15
27	Noninnocent effect of axial ligand on the heme degradation process: a theoretical approach to hydrolysis pathway of verdoheme to biliverdin. Journal of Biological Inorganic Chemistry, 2007, 13, 121-132.	2.6	15
28	A theoretical elucidation of bilirubin interaction with HSA's lysines: First electrostatic binding site in IIA subdomain. Biophysical Chemistry, 2007, 125, 375-387.	2.8	14
29	Theoretical investigations on the hydrolysis pathway of tin verdoheme complexes: elucidation of tinâ€™s ring opening inhibition role. Journal of Molecular Modeling, 2009, 15, 1299-1315.	1.8	14
30	Complexation of glycine by manganese (II) in the gas phase: A theoretical study. International Journal of Mass Spectrometry, 2010, 291, 73-83.	1.5	14
31	Comparative DFT Study To Determine if Î±-Oxoaldehydes are Precursors for Pentosidine Formation. Journal of Physical Chemistry A, 2012, 116, 2986-2996.	2.5	14
32	Carboxylated single-walled carbon nanotubes as a semiconductor for adsorption of acrylamide in mainstream cigarette smoke. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 124, 114299.	2.7	14
33	Kinetics and mechanism of the oxidation of L-Î±-amino-n-butyric acid in moderately concentrated sulfuric acid medium. Canadian Journal of Chemistry, 2004, 82, 430-436.	1.1	13
34	An ab initio/hybrid (ONIOM) investigation of biliverdin isomers and metalâ€“biliverdin analogue complexes. Computational and Theoretical Chemistry, 2003, 633, 21-33.	1.5	12
35	Towards a complete basis set limit of Hartree?Fock method: correlation-consistent versus polarized-consistent basis sets. Theoretical Chemistry Accounts, 2005, 113, 152-160.	1.4	12
36	Evaluation of the effect of the chiral centers of Taxol on binding to Î²-tubulin: A docking and molecular dynamics simulation study. Computational Biology and Chemistry, 2015, 56, 33-40.	2.3	12

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37	Tracing the Fingerprint of Chemical Bonds within the Electron Densities of Hydrocarbons: A Comparative Analysis of the Optimized and the Promolecule Densities. ChemPhysChem, 2016, 17, 3260-3268.	2.1	12
38	Semiempirical molecular orbital calculation of azobenzene: stability study of isomers and mechanism of E / Z isomerization. Computational and Theoretical Chemistry, 2000, 506, 257-261.	1.5	11
39	Prediction of novel complexation of porphine and BF3: Is it a 1:1 or 1:2 species?. Chemical Physics, 2004, 301, 1-7.	1.9	11
40	Accurate potential energy curves of Li2 and LiH: A Quantum Monte-Carlo (QMC) study. Chemical Physics Letters, 2015, 634, 101-107.	2.6	11
41	Letter to the Editor: The concept of chemical bond â€“ some like it fuzzy but others concrete. Foundations of Chemistry, 2007, 9, 85-95.	1.1	10
42	A theoretical elucidation of coordination properties of histidine and lysine to Mn2+. International Journal of Mass Spectrometry, 2012, 313, 47-57.	1.5	10
43	Comparison of the effects of sucrose molecules on alcohol dehydrogenase folding with those of sorbitol molecules on alcohol dehydrogenase folding using molecular dynamics simulation. Journal of the Iranian Chemical Society, 2015, 12, 1973-1982.	2.2	10
44	Density functional theory studies on the conversion of hydroxyheme to iron-verdoheme in the presence of dioxygen. Dalton Transactions, 2017, 46, 2146-2158.	3.3	10
45	An ab initio investigation of sulfur diimides: stability of various conformers and conformational analysis Part I. parent sulfur diimide. Computational and Theoretical Chemistry, 2003, 629, 91-104.	1.5	9
46	Theoretical studies on models of lysine-arginine cross-links derived from Î±-oxoaldehydes: a new mechanism for glucosepane formation. Journal of Molecular Modeling, 2012, 18, 1645-1659.	1.8	9
47	Interaction Modes and Absolute Affinities of Î±â€Amino Acids for Mn²⁺: A Comprehensive Picture. ChemPhysChem, 2013, 14, 1733-1745.	2.1	9
48	QM/MM Study of the Conversion of Oxophlorin into Verdoheme by Heme Oxygenase. Journal of Physical Chemistry B, 2017, 121, 11427-11436.	2.6	9
49	A novel mechanism of heme degradation to biliverdin studied by QM/MM and QM calculations. Dalton Transactions, 2018, 47, 8283-8291.	3.3	9
50	Magnetically Recyclable Fe₃O₄@TMU-32 Metalâ€“Organic Framework Photocatalyst for Tetracycline Degradation Under Visible Light. Inorganic Chemistry, 2021, 60, 17997-18005.	4.0	9
51	Theoretical studies of biliverdin: energetics of the reduction pathways to bilirubin. Journal of Molecular Modeling, 2002, 8, 113-118.	1.8	8
52	Theoretical investigation of the ring opening process of verdoheme to biliverdin in the presence of dioxygen. Journal of Molecular Modeling, 2010, 16, 1401-1413.	1.8	8
53	Theoretical calculation and prediction for experimental design to obtain spin crossover complexes. International Journal of Quantum Chemistry, 2016, 116, 1179-1186.	2.0	8
54	A benchmark study of Li2+, Li2â^', LiH+ and LiHâ^': Quantum Monte-Carlo and coupled-cluster computations. Computational and Theoretical Chemistry, 2017, 1114, 106-117.	2.5	8

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55	Effect of the axial ligands on the structure and reactivity of tin verdoheme in the ring opening process. Inorganica Chimica Acta, 2010, 363, 1577-1586.	2.4	7
56	Theoretical Study of Site Dependency on Charge Transfer at Au(111) Nanoclusters. Journal of Physical Chemistry C, 2012, 116, 5014-5018.	3.1	7
57	Separation of CH4, H2S, N2 and CO2 gases using four types of nanoporous graphene cluster model: a quantum chemical investigation. Journal of Molecular Modeling, 2021, 27, 201.	1.8	7
58	A theoretical study on the enthalpies of homolytic and heterolytic N-H bond cleavage in substituted melatonins in the gas-phase and aqueous solution. Acta Chimica Slovenica, 2013, 60, 43-55.	0.6	7
59	Semiempirical molecular orbital calculations of biliverdin: stability study of various isomers and conformation analysis. Computational and Theoretical Chemistry, 1998, 452, 125-131.	1.5	6
60	An ab initio investigation of sulfur diimides: stability of various conformers and conformational analysis part II. Dimethyl sulfur diimides (DMSD). Computational and Theoretical Chemistry, 2003, 636, 229-240.	1.5	6
61	Theoretical Investigation of Interaction of Sorbitol Molecules with Alcohol Dehydrogenase in Aqueous Solution Using Molecular Dynamics Simulation. Cell Biochemistry and Biophysics, 2011, 59, 79-88.	1.8	6
62	Complexation of nanoscale enzyme inhibitor with carbonic anhydrase active center: A quantum mechanical approach. Journal of Structural Chemistry, 2014, 55, 1574-1586.	1.0	6
63	Stoneâ€“Wales defect formation in the zigzag and armchair BC2N nanotubes: A DFT study. Physica E: Low-Dimensional Systems and Nanostructures, 2014, 58, 94-100.	2.7	6
64	A new mixed-ligand complex of copper(II) containing N-(2-pyridylmethyl)-2-pyrazinecarboxamide (NPyPzCa): Synthesis, molecular and crystal structure and properties of [Cu(NPyPzCa)(NO3)(DMSO)]. Comptes Rendus Chimie, 2011, 14, 563-567.	0.5	5
65	An in silico study on the ring-size effect in ring enlargement Bellus-Claisen rearrangement. Computational and Theoretical Chemistry, 2012, 981, 25-30.	2.5	5
66	Thermodynamic study of proton transfer in carbonic anhydrase/activator complex: A quantum mechanical approach. Computational and Theoretical Chemistry, 2013, 1022, 121-129.	2.5	5
67	Chameleonic Nature of Hydroxyheme in Heme Oxygenase and Its Reactivity: A Density Functional Theory Study. Inorganic Chemistry, 2014, 53, 2766-2775.	4.0	5
68	Theoretical study of the substituent effects on Oâ€“H BDE of trans-resveratrol derivatives in water and benzene: NBO analysis of intramolecular hydrogen bonds. Structural Chemistry, 2015, 26, 47-59.	2.0	5
69	Activation modelling of Î²- and Î³-class of carbonic anhydrase with amines and amino acids: Proton transfer process within the active site from thermodynamic point of view. Computational and Theoretical Chemistry, 2017, 1109, 42-57.	2.5	5
70	Synthesis, structural characterization, QSAR and docking studies of a new binuclear nickel (II) complex based on the flexible tetradentate N-donor ligand as a potent antibacterial and anticancer agent. International Journal of Biological Macromolecules, 2017, 104, 1107-1123.	7.5	5
71	Exploration of the binding properties of the human serum albumin sites with neurology drugs by docking and molecular dynamics simulation. Journal of the Iranian Chemical Society, 2017, 14, 19-35.	2.2	5
72	Addition of borazine to boron nitride nanotubes: [2+2] cycloaddition or bond cleavage. Monatshefte FÃ¼r Chemie, 2019, 150, 1019-1024.	1.8	5

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73	Towards developing efficient metalloporphyrin-based hybrid photocatalysts for CO2reduction; anab initiostudy. Physical Chemistry Chemical Physics, 2020, 22, 23128-23140.	2.8	5
74	An ab initio quantum chemical comparative study of possible additive rules and linear relations in parent and extended sulfur diimide families. Theoretical Chemistry Accounts, 2006, 117, 153-161.	1.4	4
75	A computational study on the mechanism and the transition states of the cyclization of 1-trifluoromethyl-1,3-dicarbonyl compounds with azides to form 1,2,3-triazoles. Computational and Theoretical Chemistry, 2014, 1043, 64-70.	2.5	4
76	Boron-nitride ad-unit and carbon ad-dimer defects in the boron nitride nanotubes. Journal of Physics and Chemistry of Solids, 2015, 79, 7-13.	4.0	4
77	Coupled Cluster and Quantum Monte-Carlo potential energy curves of the ground state of Be 2 and Be 2 + molecules. Computational and Theoretical Chemistry, 2017, 1112, 27-36.	2.5	4
78	Thiozonation and thiozonolysis of triatomic sulfur (S3) on the C70 fullerene: a DFT study. Structural Chemistry, 2018, 29, 1299-1306.	2.0	4
79	Design of new pincer fullerene ligands thorough [2+3] cycloaddition of the azomethine ylides to fullerene cage: a DFT study. Molecular Simulation, 2020, 46, 565-572.	2.0	4
80	Semiempirical molecular orbital calculations of biliverdin: study of dynamics and energetics of the self-association of a two-electron oxidation product. Computational and Theoretical Chemistry, 2000, 531, 79-88.	1.5	3
81	A theoretical investigation of electronic ground state of parent sulfur diimide. Journal of Molecular Spectroscopy, 2004, 223, 195-204.	1.2	3
82	How tin metal prevents verdoheme ring opening? Comparative study of various nucleophiles. Computational and Theoretical Chemistry, 2009, 908, 1-11.	1.5	3
83	A new chromium (III) complex containing N-(2-pyridylmethyl)-2-pyrazinecarboxamide, (NPyPzCa): Synthesis, molecular and crystal structure and theoretical electron density analysis. Solid State Sciences, 2010, 12, 1960-1965.	3.2	3
84	Kinetics and Mechanism of the Permanganate-Induced Oxidative Catalytic Condensation of Sarcosine to a Diketopiperazine. Progress in Reaction Kinetics and Mechanism, 2010, 35, 1-26.	2.1	3
85	Structure and Redox Behavior of Iron Oxophlorin and Role of Electron Transfer in the Heme Degradation Process. Inorganic Chemistry, 2012, 51, 12857-12866.	4.0	3
86	Investigation of origin of stereo-selectivity of BF3Â·Et2O-promoted allylboration of aldehydes in the presence of (R)-pinanediol by computational method. Computational and Theoretical Chemistry, 2012, 999, 28-33.	2.5	3
87	Fully and partially exohydrogenated Si80 fullerene cage: a DFT study. Structural Chemistry, 2014, 25, 575-581.	2.0	3
88	Quantum Monte Carlo simulations using Slater-Jastrow-backflow wave function. Computational and Theoretical Chemistry, 2020, 1189, 112978.	2.5	3
89	QM study of interaction between arginine amino acid and Au clusters and the effects on arginine acidity. Gold Bulletin, 2021, 54, 45-57.	2.4	3
90	An ab initio investigation of sulfur diimides: stability of conformers and conformational analysis. Part III. The effect of moieties (X) on the SN2H(X) hierarchy. Computational and Theoretical Chemistry, 2004, 673, 211-221.	1.5	2

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91	Modeling of biliverdin reduction process: regio-specificity and H-bonding. Chemical Physics, 2005, 310, 179-187.	1.9	2
92	Kinetics and mechanism of the dehydration reaction of sarcosine to a bislactame through diacyclperoxide intermediate in strong acidic medium. International Journal of Chemical Kinetics, 2009, 41, 689-703.	1.6	2
93	Conclusive evidence on the insensitivity of additive rules to the combinational details of exchange and correlation functional in hybrid DFT methods. International Journal of Quantum Chemistry, 2009, 109, 160-170.	2.0	2
94	Ab initio studies of BN-acenes and cyclo BN-acenes electronic properties and their dependence on the molecular size and the number of electrons. Computational and Theoretical Chemistry, 2009, 905, 1-7.	1.5	2
95	Synthesis of a New Class of Highly Functionalized Phosphorus Ylides Containing Heterocyclic Compounds. Chinese Journal of Chemistry, 2012, 30, 1893-1900.	4.9	2
96	Characterization of Hydrogen Bonds in the End-Functionalized Single-Wall Carbon Nanotubes: A DFT Study. Nano, 2015, 10, 1550036.	1.0	2
97	Incorporation of topological defects and atomic impurities on the carbon nanotube surface: A DFT study of ADâ€dimer defects. Heteroatom Chemistry, 2018, 29, .	0.7	2
98	QM/MM study of the conversion of biliverdin into verdoheme by heme oxygenase. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	2
99	Quantum Monte Carlo study of ground and first excited state of C, N, O, F, and Ne atoms using Slaterâ€Jastrowâ€Backflow wave function. International Journal of Quantum Chemistry, 2020, 120, e26187.	2.0	2
100	Sustainable conversion of carbon dioxide to formic acid with Rh-decorated phosphorous-doped fullerenes: a theoretical study. Structural Chemistry, 2021, 32, 97-106.	2.0	2
101	Therapeutic Effects of Static Magnetic Fields for Diabetic Wound Healing: A Review of the Current Evidence. Biosciences, Biotechnology Research Asia, 2016, 13, 353-360.	0.5	2
102	An ab initio quantum chemical study of cumulative double bonds: stability of various conformers and charge distribution analysis. Part I. XY2H2 hierarchy (X=O, S, Se and Y=N, P, As). Computational and Theoretical Chemistry, 2004, 683, 195-206.	1.5	1
103	Linear regression analysis of molecular energy properties for poly heterocyclic compounds. Computational and Theoretical Chemistry, 2009, 906, 35-40.	1.5	1
104	Kinetics and Mechanism of the Kmn04-Oxidative Catalysed Condensation Reaction of L-Proline to a Diketopiperazine: Evidence for Delayed Autocatalytic Behaviour. Progress in Reaction Kinetics and Mechanism, 2011, 36, 95-119.	2.1	1
105	Kinetics and Mechanism of the Permanganate-Induced Autocatalytic Dehydration Reaction of L-Y-Amino-N-Butyric Acid to Give 2-Pyrrolidone through a Radical Intermediate in Moderately Concentrated Acidic Medium. Progress in Reaction Kinetics and Mechanism, 2011, 36, 120-138.	2.1	1
106	QM study of complexation between natural bilirubin and poly-terthiophene carboxylic acidâ€“Mn(II) as a biosensor: Temperature and interferences effect. Journal of Theoretical and Computational Chemistry, 2015, 14, 1550048.	1.8	1
107	The Theoretical and Experimental Studies on Oxidation of Straight Chain Amino Acids in Moderately Concentrated Sulfuric Acid Medium. International Journal of Chemical Kinetics, 2016, 48, 647-659.	1.6	1
108	Theoretical study on the mono and multiply oxygenated Si₆₀H₆₀ fullerene. Molecular Physics, 2016, 114, 819-828.	1.7	1

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109	AlSi2P nanotubes: a theoretical study. Structural Chemistry, 2016, 27, 525-533.	2.0	1
110	Computational study for the circular redox reaction of N2O with CO catalyzed by fullerometallic cations C60Fe+ and C70Fe+. Journal of Molecular Graphics and Modelling, 2017, 72, 50-57.	2.4	1
111	Chlorofluorofullerenes (CFFs). Structural Chemistry, 2017, 28, 1707-1716.	2.0	1
112	Polarizability of the Si60H60 Derivatives Containing Epoxide Moieties (Si60H60â^'2nOn with n up to 30): A DFT Study. Journal of Cluster Science, 2018, 29, 889-896.	3.3	1
113	Formation of boron nitride islands in the graphene nanoflakes: A DFT study. Materials Chemistry and Physics, 2019, 223, 164-170.	4.0	1
114	Coupled Cluster and Quantum Monte-Carlo study of anionic hydrogen clusters <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si27.svg"><mml:mrow><mml:msubsup><mml:mi mathvariant="normal">H</mml:mi><mml:mrow><mml:mi>n</mml:mi></mml:mrow><mml:mo>-</mml:mo></mml:msubsup><mml:mfe close="		

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127	Computational Design of New Hydroborane Fullerene-Based Pincer Ligands. Journal of Cluster Science, 0, , 1.	3.3	0
128	Computational Design of New N-Heterocyclic Silyl Pincer Fullerenes. Silicon, 0, , 1.	3.3	0
129	Theoretical exploration of the LiF-decorated BN cages as hydrogen storage materials. Monatshefte FÃ¼r Chemie, 2021, 152, 931-938.	1.8	0
130	The effect of external electric field and metal impurities on the interaction of HF and boraphene: a computational study. Journal of Molecular Modeling, 2021, 27, 50.	1.8	0