Saeed Jamehbozorgi

List of Publications by Year
in descending order

65	746	567144 15	610775 24
papers	citations	h-index	g-index

65	65	65	629
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Prediction of toxicity of nitrobenzenes using ab initio and least squares support vector machines. Journal of Hazardous Materials, 2008, 151, 603-609.	6.5	65
2	Warped C 80 H 30 nanographene as a chemical sensor for CO gas: DFT studies. Physics Letters, Section A: General, Atomic and Solid State Physics, 2017, 381, 646-651.	0.9	51
3	Ab initio study of the structures and dynamic stereochemistry of biaryls. Computational and Theoretical Chemistry, 2005, 717, 41-51.	1.5	45
4	DFT/TD-semiempirical study on the structural and electronic properties and absorption spectra of supramolecular fullerene-porphyrine-metalloporphyrine triads based dye-sensitized solar cells. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 194, 57-66.	2.0	40
5	A comparative study of structural and electronic properties of formaldehyde molecule on monolayer honeycomb structures based on vdW-DF prospective. Applied Surface Science, 2016, 384, 175-181.	3.1	34
6	The effect of water on the electronic and field emission properties of inorganic AlN nanocones: Computational study. Inorganic Chemistry Communication, 2018, 90, 86-91.	1.8	27
7	Understanding delivery and adsorption of Flutamide drug with ZnONS based on: Dispersion-corrected DFT calculations and MD simulations. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 135, 114937.	1.3	27
8	The Role of Polyethylene Glycol Size in Chemical Spectra, Cytotoxicity, and Release of PEGylated Nanoliposomal Cisplatin. Assay and Drug Development Technologies, 2019, 17, 231-239.	0.6	25
9	DFT study and NBO analysis of the mutual interconversion of cumulene compounds. Journal of Physical Organic Chemistry, 2007, 20, 355-364.	0.9	21
10	Solvent effect on the linkage isomerism in [Fe(CO)₄(NCS)]^{â^'}and [Fe(CO)₄(SCN)]^{â^'}anions: A theoretical investigation. Physics and Chemistry of Liquids, 2017, 55, 444-456.	0.4	20
11	Solvent Effects on the Structure And Spectroscopic Properties of the Second-Generation Anticancer Drug Carboplatin: A Theoretical Insight. Journal of Structural Chemistry, 2018, 59, 245-251.	0.3	20
12	Synthesis and characterization of a new poly(Nâ€“heterocyclic carbene Cu complex) immobilized on nanoâ€“silica, (CuIIâ€“NHCs)n@nSiO2, and its application as an efficient and reusable catalyst in the synthesis of benzimidazoles, benzothiazoles, 1,2,3â€“triazoles, bisâ€“triazoles and sonogashiraâ€“hagihara reactions. Inorganica Chimica Acta, 2019, 485, 173-189.	1.2	20
13	Quantum Chemical Study of the Solvent Effect on the Anticancer Active Molecule of Iproplatin: Structural, Electronic, and Spectroscopic Properties (IR, 1H NMR, UV). Journal of Applied Spectroscopy, 2017, 83, 909-916.	0.3	19
14	Computational study of osmabenzyne: The solvent effects on the structure and spectroscopic properties (IR, NMR). Journal of Structural Chemistry, 2017, 58, 1324-1331.	0.3	18
15	Structural and electronic properties of metalloporphyrin (MP, M = Fe, Co and Zn) adsorbed on single walled BNNT and SiCNT. Applied Surface Science, 2016, 360, 69-76.	3.1	17
16	Assessing of Removal Efficiency of Indigo Carmine from Wastewater Using MWCNTs. Iranian Journal of Science and Technology, Transaction A: Science, 2017, 41, 1047-1053.	0.7	16
17	Synthesis of 1â€amidoalkylâ€2â€naphthol derivatives using a magnetic nanoâ€Fe₃O₄@SiO₂@Hexamethylenetetramineâ€supported ionic liquid as a catalyst under solventâ€free conditions. Journal of the Chinese Chemical Society, 2020, 67, 603-609.	0.8	15
18	A new type of heteroborospherene as a versatile carrier for drug delivery: A theoretical study. Physica E: Low-Dimensional Systems and Nanostructures, 2020, 117, 113852.	1.3	15

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19	Theoretical Study of Substituent Effects on Geometric and Spectroscopic Parameters (IR,¹³C,²⁹Si NMR) and Energy Decomposition Analysis of the Bonding in Molybdenum Silylidyne Complexes CpMo(CO)₂(â‰¡Si-para-C₆H₄X). Journal of the Chinese Chemical Society, 2017, 64, 522-530.	0.8	14
20	Influence of Solvent and Electric Field on the Structure and IR, 31P NMR Spectroscopic Properties of a Titanoceneâ€“Benzyne Complex. Journal of Applied Spectroscopy, 2018, 85, 526-534.	0.3	14
21	Adsorption of Cd and Ni from water by graphene oxide and graphene oxideâ€“almond shell composite. Water Environment Research, 2019, 91, 475-482.	1.3	13
22	Microfunnelâ€filterâ€based emulsification microextraction followed by gas chromatography for simple determination of organophosphorus pesticides in environmental water samples. Journal of Separation Science, 2019, 42, 2418-2425.	1.3	13
23	Î³-graphyne and its boron nitride analogue as nanocarriers for anti-cancer drug delivery. Molecular Physics, 2020, 118, e1691748.	0.8	13
24	Electrochemical Synthesis of 4-(Dihydroxyphenylthio)-2H-chromen-2-one Derivatives. Chemical and Pharmaceutical Bulletin, 2008, 56, 1562-1566.	0.6	11
25	The effect of encapsulation of lithium atom on supramolecular triad complexes performance in solar cell by using theoretical approach. Adsorption, 2020, 26, 471-489.	1.4	11
26	Theoretical study on the electronic, structural, properties and reactivity of a series of mono-, di-, tri- and tetrafluorothiophenes as monomers for new conducting polymers. Journal of Fluorine Chemistry, 2011, 132, 190-195.	0.9	10
27	Synthesis, characterization, spectroscopic study, and catalytic behavior of ruthenium(II) o-phenanthroline complex with dipicolinate. Journal of Coordination Chemistry, 2012, 65, 994-1003.	0.8	10
28	Effect of the External Electric Field on the Electronic Structure and Aromaticity of Iridabenzene: A DFT Study. Journal of Structural Chemistry, 2019, 60, 547-555.	0.3	10
29	The interaction of 5-fluorouracil with graphene in presence of external electric field: a theoretical investigation. Adsorption, 2020, 26, 905-911.	1.4	10
30	Preparation of nanostructured Coâ€“Mo alloy electrodes and investigation of their electrocatalytic activity for hydrazine oxidation in alkaline medium. Journal of the Chinese Chemical Society, 2018, 65, 970-976.	0.8	9
31	Tandem dispersive liquidâ€“liquid microextraction coupled with micro-sampling flame atomic absorption spectrometry for rapid determination of lead(II) and cadmium(II) ions in environmental water samples. International Journal of Environmental Analytical Chemistry, 2019, 99, 1235-1246.	1.8	9
32	Nickel(II) catalyzed oxidation of aldehyde derivatives to their carboxylic acid or ester analogs. Research on Chemical Intermediates, 2013, 39, 3319-3325.	1.3	8
33	Preparation of CoFe₂O₄/sawdust and NiFe₂O₄/sawdust magnetic nanocomposites for removal of oil from the water surface. Journal of the Chinese Chemical Society, 2020, 67, 288-297.	0.8	8
34	An Ab Initio Study and NBO Analysis of the Stability and Conformational Properties of Hexakis(trimethylelementhyl)benzene (Element = C, Si, Ge, and Sn). Phosphorus, Sulfur and Silicon and the Related Elements, 2006, 181, 2419-2434.	0.8	7
35	Structural, energetic and electrical properties of encapsulation of penicillamine drug into the CNTs based on vdW-DF perspective. Physica E: Low-Dimensional Systems and Nanostructures, 2015, 72, 120-127.	1.3	7
36	Analysis of the Interaction Between the C20 Cage and cis-Ptcl2(NH3)2: A DFT Investigation of the Solvent Effect, Structures, Properties, and Topologies. Journal of Structural Chemistry, 2018, 59, 1044-1051.	0.3	7

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37	Ab Initio Study of Structures, Metallotropic 1,2-Shifts and Prototropic 1,2-Shifts of Cyclopentadienyl(trimethyl)silane, -germane and -stannane. Phosphorus, Sulfur and Silicon and the Related Elements, 2003, 178, 341-351.	0.8	6
38	Ab Initio and NBO Studies of the Decomposition ([2+2] and [2+4]Elimination) Mechanisms of Alkylisothiocyanates (alkyl = ethyl-, iso-propyl- and tert-butyl). Phosphorus, Sulfur and Silicon and the Related Elements, 2006, 181, 75-85.	0.8	6
39	Ab Initio Study of Geminal Steric Hindrance Effects on the Stability of Conformations of Cyclohexane Derivatives. Journal of Chemical Research, 2005, 2005, 508-515.	0.6	5
40	Ab Initio Study of Ring Flipping of the Overcrowded Peri-Substituted Naphthalenes. Phosphorus, Sulfur and Silicon and the Related Elements, 2003, 178, 2529-2537.	0.8	4
41	Quantitative structureâ€“property relationship study of the solubility of thiazolidine-4-carboxylic acid derivatives using ab initio and genetic algorithmâ€“partial least squares. Chinese Chemical Letters, 2007, 18, 621-624.	4.8	4
42	Simultaneous Voltammetric Determination of Lead and Tin by Adsorptive Differential Pulse Stripping Method and Orthogonal Signal Correctionâ€Partial Least Squares in Water Samples. Journal of the Chinese Chemical Society, 2008, 55, 276-285.	0.8	4
43	Theoretical study on the electronic, structural, properties and reactivity of a series of mono-, di-, tri- and tetrachlorothiophenes as well as corresponding radical cation forms as monomers for conducting polymers. Chemistry Central Journal, 2011, 5, 13.	2.6	4
44	Cytotoxicity of Nanoliposomal Cisplatin Coated with Synthesized Methoxypolyethylene Glycol Propionaldehyde in Human Ovarian Cancer Cell Line A2780CP. Tropical Journal of Pharmaceutical Research, 2016, 15, 563.	0.2	4
45	A Computational Approach for Hydrolysis of the Third-Generation Anticancer Drug: Trans-Platinum(Ii) Complex of 3-Aminoflavone. Journal of Structural Chemistry, 2018, 59, 1791-1796.	0.3	4
46	Enhancing Photocatalytic Activity of Cu2O in Degradation of Sulphonic Acid-Based Dye. Russian Journal of Applied Chemistry, 2019, 92, 141-149.	0.1	4
47	Synthesis of Tetrazoles Catalyzed by Novel Cobalt Magnetic Nanoparticles. Russian Journal of Organic Chemistry, 2019, 55, 1777-1784.	0.3	4
48	The Role of Pseudo Jahnâ€“Teller Effect in Geometry and Electronic Parameters of Tetrahalodigermene Ge2X4 (X= Cl, Br, I). Russian Journal of Physical Chemistry A, 2019, 93, 1297-1304.	0.1	3
49	Selective and Sensitive Two New Macroacyclic Schiff base Fluorescent Turnâ€Off Receptors for Fe³⁺, DFT Calculation and Their Antibacterial Activity. Applied Organometallic Chemistry, 2020, 34, e5430.	1.7	3
50	Ab initio Study of Configurational and Conformational Properties of Cyclodeca-1,2,4,6,7,9-Hexaene and Cyclodeca-1,2,4,6,8,9-Hexaene^{â€}. Journal of Chemical Research, 2003, 2003, 384-385.	0.6	2
51	Synthesis, Characterization, and an ab initio Study of a Manganese(II) Macrocyclic Schiff-Base Complex with Two 2-Aminoethyl Pendant Arms. Transition Metal Chemistry, 2004, 29, 523-527.	0.7	2
52	Theoretical Study of Substituent Effect on the Electronic and Optical Properties of 4-Substituted Ferrocenylethynylbenzenes. Russian Journal of Physical Chemistry A, 2019, 93, 1747-1753.	0.1	2
53	Hybrid-DFT Study and NBO Interpretation of the Configurational Behavior of 2-Halotetrahydrothiopyran S-Oxides. Phosphorus, Sulfur and Silicon and the Related Elements, 2013, 188, 839-849.	0.8	1
54	Facile, low-cost, and organic-free fabrication of diverse nanoporous alumina as support for drug release; on the salt effect, calcination temperature, and reaction time dependence. Journal of Sol-Gel Science and Technology, 2017, 83, 627-639.	1.1	1

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55	Hydrothermal synthesis of a dinuclear copper(II) complex with 2-aminopyrimidine and bridging oxalate ligands: in situ degradation of tartaric acid to oxalate and thermal decomposition to CuO nanoparticles. Inorganic and Nano-Metal Chemistry, 2020, 50, 1353-1357.	0.9	1
56	<i>Ab initio</i> and DFT Study of Prototropic and Metallotropic 1,5-Shifts of Isolobal Cyclopentadienyl Derivatives. Current Science, 2017, 112, 743.	0.4	1
57	Investigation of Interaction Between Graphene and Its Compounds as Carriers on Anti-Cancer Drug of 5-Fluorouracil. Eurasian Journal of Analytical Chemistry, 2018, 13, .	0.4	1
58	Computational study of substituent effect on the electronic properties of ferrocylidene acetophenones complexes. Eurasian Chemical Communications, 2019, 1, 411-418.	1.1	1
59	Ab initio Study of Configurations of Cycloundeca-1,2,4,5,7,8,10-heptaene. Journal of Chemical Research, 2002, 2002, 544-546.	0.6	0
60	Ab Initio Study of Conformational Properties of (Z,Z,Z)-Cyclonona-1,3,6-Triene. Journal of Chemical Research, 2003, 2003, 546-548.	0.6	0
61	Ab initio study of the conformational properties of (Z,Z)-cyclodeca-1,6-diene and its heterocyclic analogue containing oxygen. Computational and Theoretical Chemistry, 2005, 716, 211-215.	1.5	0
62	Ab Initio Study of the Various Pathways of the Decomposition ([2+2]elimination) of 2-Chloroethyltrichlorosilane. Phosphorus, Sulfur and Silicon and the Related Elements, 2005, 180, 1611-1619.	0.8	0
63	Keto-enol tautomerism in estrogen hormone. A theoretical study. , 2015, , .		0
64	DFT studies of all fluorothiophenes and their cations as candidate monomers for conductive polymers. , 2015, , .		0
65	THEORETICAL STUDY OF THE PH3-ASSISTED MIGRATION OF A COORDINATED ARYL GROUP TO A COORDINATED CO IN THE COMPLEXES RhCpI(CO)(p-XC6H4). Journal of the Chilean Chemical Society, 2017, 62, 3454-3461.	0.5	0