Saeed Jamehbozorgi

List of Publications by Citations

59 papers	493 citations	12 h-index	18 g-index
65 ext. papers	609 ext. citations	2.1 avg, IF	4.25 L-index

#	Paper	IF	Citations
59	Prediction of toxicity of nitrobenzenes using ab initio and least squares support vector machines. *Journal of Hazardous Materials*, **2008**, 151, 603-9	12.8	59
58	Ab initio study of the structures and dynamic stereochemistry of biaryls. *Computational and Theoretical Chemistry*, **2005**, 717, 41-51		38
57	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	2.3	25
56	Solvent effect on the linkage isomerism in [Fe(CO)4(NCS)]− and [Fe(CO)4(SCN)]− anions: A theoretical investigation. *Physics and Chemistry of Liquids*, **2017**, 55, 444-456	1.5	20
55	DFT study and NBO analysis of the mutual interconversion of cumulene compounds. *Journal of Physical Organic Chemistry*, **2007**, 20, 355-364	2.1	20
54	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	0.7	19
53	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	0.9	18
52	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	6.7	18
51	Computational study of osmabenzyne: The solvent effects on the structure and spectroscopic properties (IR, NMR). *Journal of Structural Chemistry*, **2017**, 58, 1324-1331	0.9	17
50	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(?Si-para-C6H4X). *Journal of the Chinese Chemical Society*, **2017**, 64, 522-530	1.5	14
49	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	2.1	13
48	Influence of Solvent and Electric Field on the Structure and IR, 31P NMR Spectroscopic Properties of a Titanocene–Benzyne Complex. *Journal of Applied Spectroscopy*, **2018**, 85, 526-534	0.7	13
47	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	4.4	12
46	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	6.7	11
45	Synthesis and characterization of a new poly(N-heterocyclic carbene Cu complex) immobilized on nano-silica, (CuI-NHCs)n@nSiO2, and its application as an efficient and reusable catalyst in the synthesis of benzimidazoles, benzothiazoles, 1,2,3-triazoles, bis-triazoles and Sonogashira–Hagihara reactions. *Inorganica Chimica Acta*, **2019**, 485, 173-183	2.7	11
44	Synthesis, characterization, spectroscopic study, and catalytic behavior of ruthenium(II) o-phenanthroline complex with dipicolinate. *Journal of Coordination Chemistry*, **2012**, 65, 994-1003	1.6	10
43	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	3	10

42	Adsorption of Cd and Ni from water by graphene oxide and graphene oxide-almond shell composite. *Water Environment Research*, **2019**, 91, 475-482	2.8	9
41	Microfunnel-filter-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	3.4	9
40	The effect of water on the electronic and field emission properties of inorganic AlN nanocones: Computational study. *Inorganic Chemistry Communication*, **2018**, 90, 86-91	3.1	9
39	Assessing of Removal Efficiency of Indigo Carmine from Wastewater Using MWCNTs **2017**, 41, 1047-1053		8
38	Electrochemical synthesis of 4-(dihydroxyphenylthio)-2H-chromen-2-one derivatives. *Chemical and Pharmaceutical Bulletin*, **2008**, 56, 1562-6	1.9	8
37	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	2.1	7
36	Synthesis of 1-amidoalkyl-2-naphthol derivatives using a magnetic nano-Fe3O4@SiO2@Hexamethylenetetramine-supported ionic liquid as a catalyst under solvent-free conditions. *Journal of the Chinese Chemical Society*, **2020**, 67, 603-609	1.5	7
35	Tandem dispersive liquid□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	6
34	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	2	6
33	Nickel(II) catalyzed oxidation of aldehyde derivatives to their carboxylic acid or ester analogs. *Research on Chemical Intermediates*, **2013**, 39, 3319-3325	2.8	6
32	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	1	6
31	□graphyne and its boron nitride analogue as nanocarriers for anti-cancer drug delivery. *Molecular Physics*, **2020**, 118, e1691748	1.7	6
30	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	0.9	5
29	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	1	5
28	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
27	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	3	5
26	Enhancing Photocatalytic Activity of Cu2O in Degradation of Sulphonic Acid-Based Dye. *Russian Journal of Applied Chemistry*, **2019**, 92, 141-149	0.8	4
25	Preparation of nanostructured Co□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	1.5	4

24	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		4
23	Simultaneous Voltammetric Determination of Lead and Tin by Adsorptive Differential Pulse Stripping Method and Orthogonal Signal Correction-Partial Least Squares in Water Samples. *Journal of the Chinese Chemical Society*, **2008**, 55, 276-285	1.5	4
22	Quantitative structure□property relationship study of the solubility of thiazolidine-4-carboxylic acid derivatives using ab initio and genetic algorithm□partial least squares. *Chinese Chemical Letters*, **2007**, 18, 621-624	8.1	4
21	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	1	4
20	The interaction of 5-fluorouracil with graphene in presence of external electric field: a theoretical investigation. *Adsorption*, **2020**, 26, 905-911	2.6	4
19	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	0.9	4
18	Ab Initio Study of Ring Flipping of the Overcrowded Peri-Substituted Naphthalenes. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2003**, 178, 2529-2537	1	3
17	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	1.5	3
16	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	0.9	3
15	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	0.7	2
14	Selective and Sensitive Two New Macroacyclic Schiff base Fluorescent Turn-Off Receptors for Fe3+, DFT Calculation and Their Antibacterial Activity. *Applied Organometallic Chemistry*, **2020**, 34, e5430	3.1	2
13	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□*Journal of Chemical Research*, **2003**, 2003, 384-385	0.6	2
12	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	2.1	2
11	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	0.8	2
10	The Role of Pseudo Jahn□Teller Effect in Geometry and Electronic Parameters of Tetrahalodigermene Ge2X4 (X= Cl, Br, I). *Russian Journal of Physical Chemistry A*, **2019**, 93, 1297-1304	0.7	1
9	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	2.3	1
8	Synthesis of Tetrazoles Catalyzed by Novel Cobalt Magnetic Nanoparticles. *Russian Journal of Organic Chemistry*, **2019**, 55, 1777-1784	0.7	1
7	The effect of encapsulation of lithium atom on supramolecular triad complexes performance in solar cell by using theoretical approach. *Adsorption*, **2020**, 26, 471-489	2.6	1

6	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	1.2	0
5	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	1	0
4	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	
3	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		
2	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	1	
1	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	