

Ali Morsali

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

86
papers

942
citations

17
h-index

26
g-index

87
ext. papers

1,096
ext. citations

2.9
avg, IF

4.82
L-index

#	Paper	IF	Citations
86	New regularities and an equation of state for liquids. <i>Fluid Phase Equilibria</i> , 2005 , 230, 170-175	2.5	60
85	Assessment of the adsorption mechanism of Flutamide anticancer drug on the functionalized single-walled carbon nanotube surface as a drug delivery vehicle: An alternative theoretical approach based on DFT and MD. <i>Applied Surface Science</i> , 2018 , 434, 492-503	6.7	57
84	Mechanism and Kinetics of the Wacker Process: A Quantum Mechanical Approach. <i>Organometallics</i> , 2008 , 27, 72-79	3.8	56
83	Theoretical study of solvent and co-solvent effects on the interaction of Flutamide anticancer drug with Carbon nanotube as a drug delivery system. <i>Journal of Molecular Liquids</i> , 2017 , 248, 490-500	6	46
82	S-allyl-3-(2-pyridyl-methylene)dithiocarbazate ligand and its manganese(II), cobalt(III) and nickel(II) complexes. <i>Inorganica Chimica Acta</i> , 2011 , 371, 36-41	2.7	37
81	Synthesis, experimental and theoretical characterization of tetra dentate N,NRdipyridoxyl (1,3-propylenediamine) salen ligand and its Co(III) complex. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2008 , 71, 1341-7	4.4	37
80	An accurate expression for radial distribution function of the Lennard-Jones fluid. <i>Chemical Physics</i> , 2005 , 310, 11-15	2.3	36
79	N,NRdipyridoxyl Schiff bases: synthesis, experimental and theoretical characterization. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011 , 83, 467-71	4.4	35
78	Assessment of solvent effects on the interaction of Carmustine drug with the pristine and COOH-functionalized single-walled carbon nanotubes: A DFT perspective. <i>Journal of Molecular Liquids</i> , 2017 , 240, 87-97	6	31
77	Quantum chemical studies of chitosan nanoparticles as effective drug delivery systems for 5-fluorouracil anticancer drug. <i>Journal of Molecular Liquids</i> , 2020 , 302, 112495	6	30
76	H-Transfer steps of the Wacker process: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2009 , 903, 108-114		29
75	Synthesis, experimental and theoretical characterizations of a new Schiff base derived from 2-pyridincarboxaldehyde and its Ni (II) complex. <i>Journal of Molecular Structure</i> , 2017 , 1143, 424-430	3.4	26
74	Comprehensive quantum chemical insight into the mechanistic understanding of the surface functionalization of carbon nanotube as a nanocarrier with cladribine anticancer drug. <i>Applied Surface Science</i> , 2018 , 462, 720-729	6.7	24
73	Synthesis, experimental and theoretical characterization of a Mn(II) complex of N,N?-dipyridoxyl(1,2-diaminobenzene). <i>Journal of Molecular Structure</i> , 2017 , 1127, 15-22	3.4	20
72	The computational study of the EFeO nanoparticle as Carmustine drug delivery system: DFT approach. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019 , 37, 454-464	3.6	19
71	Theoretical Study of Solvent Effects on the Cis-to-Trans Isomerization of [Pd(C6Cl2F3)I(PH3)2]. <i>Journal of Solution Chemistry</i> , 2013 , 42, 1902-1911	1.8	18
70	Extraordinary catalytic activity of a Keplerate-type giant nanoporous isopolyoxomolybdate in the synthesis of 1,8-dioxo-octahydroxanthenes and 1,8-dioxodecahydroacridines. <i>Research on Chemical Intermediates</i> , 2015 , 41, 7815-7826	2.8	17

69	OH bond cleavage step of the Wacker process: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2010 , 941, 138-143		17
68	Three VO ₂ ⁺ complexes of the pyridoxal-derived Schiff bases: Synthesis, experimental and theoretical characterizations, and catalytic activity in a cyclocondensation reaction. <i>Journal of Molecular Structure</i> , 2018 , 1153, 149-156	3.4	16
67	Quantum mechanical study on the mechanism and kinetics of the cis-to-trans isomerization of [Pd(C ₆ Cl ₂ F ₃)I(PH ₃) ₂]. <i>Inorganica Chimica Acta</i> , 2013 , 394, 423-429	2.7	16
66	Quantum mechanical study on the mechanism and kinetics of the hydrolysis of organopalladium Complex [Pd(CNN)P(OMe) ₃] ⁺ in low acidity range. <i>Computational and Theoretical Chemistry</i> , 2012 , 994, 41-46	2	16
65	Molecular mechanism study of surface functionalization of silica nanoparticle as an anticancer drug nanocarrier in aqueous solution. <i>Journal of Molecular Liquids</i> , 2019 , 282, 392-400	6	15
64	A DFT investigation of structure, spectroscopic properties and tautomerism of the anticonvulsant drug Lyrica. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015 , 138, 637-42	4.4	15
63	A molecular dynamics study on the role of attractive and repulsive forces in internal energy, internal pressure and structure of dense fluids. <i>Chemical Physics</i> , 2007 , 331, 332-338	2.3	15
62	Theoretical and Experimental Studies on the Regioselectivity of Epoxide Ring Opening by Nucleophiles in Nitromethane without any Catalyst: Nucleophilic-Chain Attack Mechanism. <i>Progress in Reaction Kinetics and Mechanism</i> , 2014 , 39, 89-102	0.5	14
61	Mechanism of the Formation of Palladium(II) Maleate Complex: A DFT Approach. <i>International Journal of Chemical Kinetics</i> , 2015 , 47, 73-81	1.4	13
60	Synthesis, characterization and intramolecular proton transfer of 3,3'-dihydroxy-4,4'-[5-methyl-1,3-phenylenebis(nitrilomethylidyne)]-bis-phenol. <i>Journal of Molecular Structure</i> , 2014 , 1072, 187-194	3.4	13
59	Treatment of the breast cancer by using low frequency electromagnetic fields and Mn(II) complex of a Schiff base derived from the pyridoxal. <i>Breast</i> , 2018 , 41, 107-112	3.6	12
58	DFT study of SiO ₂ nanoparticles as a drug delivery system: structural and mechanistic aspects. <i>Structural Chemistry</i> , 2019 , 30, 715-726	1.8	12
57	Synthesis, experimental and theoretical characterizations of a 1,2,4-triazole Schiff base and its nickel(II) complex. <i>Journal of Molecular Structure</i> , 2019 , 1179, 779-786	3.4	11
56	Quantum chemical modeling of iron oxide magnetic nanoparticles functionalized with cytarabine. <i>Chemical Physics Letters</i> , 2019 , 719, 12-21	2.5	9
55	Synthesis, experimental and computational characterizations of a new quinoline derived Schiff base and its Mn(II), Ni(II) and Cu(II) complexes. <i>Journal of Molecular Structure</i> , 2020 , 1208, 127898	3.4	9
54	Evaluation of PVT differential properties of the Lennard-Jones fluid using radial distribution functions and molecular dynamics. <i>Chemical Physics</i> , 2007 , 335, 194-200	2.3	9
53	Surface functionalization of chitosan with 5-nitroisatin. <i>International Journal of Biological Macromolecules</i> , 2020 , 147, 534-546	7.9	9
52	QTAIM study of substituent effects on the intramolecular hydrogen bond in 3,3'-dihydroxy-4,4'-[5-methyl-1,3-phenylenebis(nitrilomethylidyne)]-bis-phenol. <i>Journal of Molecular Structure</i> , 2015 , 1083, 1-9	3.4	8

51	Experimental and Theoretical Studies on the Tautomerism in 2-Aminopyridines and 2(1H)-Pyridinones: Synthesis of 2-Amino-4-aryl-3-cyano-6-(3,4-dimethoxyphenyl)pyridines and 4-Aryl-3-cyano-6-(3,4-dimethoxyphenyl)-2(1H)-pyridinones. <i>Bulletin of the Korean Chemical Society</i> , 2011 , <i>32</i> , 1873-1878	1.2	8
50	Theoretical Investigation on the Kinetics and Mechanism of the Synthesis of Fluorescent 3,8-Disubstituted-3H-Imidazo [4,5-a] Acridine-11-Carbonitriles. <i>Progress in Reaction Kinetics and Mechanism</i> , 2016 , <i>41</i> , 365-370	0.5	8
49	Quantum mechanical study of the alkoxide-independent pathway of reductive elimination of CO from palladium (p-cyanophenyl) neopentoxide complex. <i>Research on Chemical Intermediates</i> , 2015 , <i>41</i> , 5389-5398	2.8	7
48	Stability appraisalment of the alumina-brine nanofluid in the presence of ionic and non-ionic dispersants on the alumina nanoparticles surface as heat transfer fluids: Quantum mechanical study and Taguchi-optimized experimental analysis. <i>Journal of Molecular Liquids</i> , 2020 , <i>319</i> , 113898	6	7
47	Density functional theory study towards investigating the adsorption properties of the Fe ₂ O ₃ nanoparticles as a nanocarrier for delivery of Flutamide anticancer drug. <i>Adsorption</i> , 2020 , <i>26</i> , 925-939	2.6	7
46	Synthesis, experimental and DFT characterization of the 2-((E)-(2-[(E)-2,3-Dihydroxybenzylideneamino]-5-methylphenyl)imino)methyl)-6-hydroxyphenolate and its Ni(II) and Cu(II) complexes. <i>Journal of Molecular Structure</i> , 2017 , <i>1146</i> , 620-628	3.4	6
45	Quantum Mechanical Study of Fe ₂ O ₃ Nanoparticle as a Nanocarrier for Anticancer Drug Delivery. <i>Zeitschrift Fur Physikalische Chemie</i> , 2018 , <i>232</i> , 579-592	3.1	6
44	Green synthesis of zinc oxide and copper oxide nanoparticles using <i>Achillea Nobilis</i> extract and evaluating their antioxidant and antibacterial properties. <i>Bulletin of Materials Science</i> , 2021 , <i>44</i> , 1	1.7	6
43	The effect of different alcohols on the Asp23-Lys28 and Asp23-Ala42 salt bridges of the most effective peptide in Alzheimer's disease: Molecular dynamics viewpoints. <i>Journal of Molecular Graphics and Modelling</i> , 2019 , <i>86</i> , 199-208	2.8	6
42	Quantum Mechanical Study on the Mechanistic, Energetic, and Structural Properties of Adsorption of 6-Thioguanine onto Fe ₂ O ₃ Nanoparticles. <i>Bulletin of the Korean Chemical Society</i> , 2017 , <i>38</i> , 869-874	1.2	5
41	The study of self-aggregation behavior of the bilirubin molecules in the presence and absence of carbon nanotubes: Molecular dynamics simulation approach. <i>Journal of Molecular Liquids</i> , 2015 , <i>208</i> , 342-346	6	5
40	The sound velocities in dense fluids from distribution functions. <i>Physics and Chemistry of Liquids</i> , 2010 , <i>48</i> , 50-61	1.5	5
39	Comprehension of the role of created hydrogen bonds and adsorption energy in polyamide-nanosilica- Keggin hybrid/ water on enhancement of concrete compressive strength: DFT calculations and experimental investigations. <i>Journal of Molecular Liquids</i> , 2020 , <i>297</i> , 111912	6	5
38	Does high pressure have any effect on the structure of alpha amylase and its ability to binding to the oligosaccharides having 3-7 residues? Molecular dynamics study. <i>Journal of Molecular Graphics and Modelling</i> , 2018 , <i>80</i> , 85-94	2.8	4
37	THE HEAT CAPACITIES FROM ANALYTICAL DISTRIBUTION FUNCTIONS. <i>Journal of Theoretical and Computational Chemistry</i> , 2009 , <i>08</i> , 943-956	1.8	4
36	The changes in free energies and entropies from analytical radial distribution functions. <i>Physics and Chemistry of Liquids</i> , 2012 , <i>50</i> , 187-198	1.5	4
35	A density functional theory investigation of the bromide oxidation mechanism by a vanadium bromoperoxidase model complex. <i>Transition Metal Chemistry</i> , 2010 , <i>35</i> , 939-947	2.1	4
34	Quantum molecular study of mesoporous silica nanoparticle as a delivery system for troxacitabine anticancer drug. <i>Journal of Molecular Liquids</i> , 2020 , <i>310</i> , 113155	6	3

33	A molecular dynamics study on the role of attractive and repulsive forces in excess heat capacity at constant volume of dense fluids. <i>Molecular Physics</i> , 2012 , 110, 483-490	1.7	3
32	Investigation into the Regiochemistry of Some Pyrazoles Derived from 1,3-Dipolar Cycloaddition of Methyl Methacrylate with Some Nitrilimines: A Combined Theoretical and Experimental Study. <i>Chinese Journal of Chemistry</i> , 2011 , 29, 1167-1172	4.9	3
31	Role of repulsive forces on self-assembly behavior of amyloid peptide (1-40): Molecular dynamics simulation approach. <i>Physica A: Statistical Mechanics and Its Applications</i> , 2019 , 513, 524-535	3.3	3
30	Density Functional Theoretical Study on the Mechanism of Alcoholysis of Acylpalladium(II) Complexes. <i>Progress in Reaction Kinetics and Mechanism</i> , 2017 , 42, 52-61	0.5	2
29	Kinetics and mechanism of producing 3,8-dimethyl-3H-imidazo[4,5-a]acridine-11-carbonitrile: a DFT investigation. <i>Research on Chemical Intermediates</i> , 2017 , 43, 1829-1846	2.8	2
28	A molecular dynamics study on the role of attractive and repulsive forces in isobaric heat capacity and sound velocity of sub- and supercritical dense fluids. <i>Journal of Supercritical Fluids</i> , 2014 , 95, 628-634	4.2	2
27	Synthesis and characterisation of modified carbon nanotubes with potassium salts of the monosubstituted Keggin polyoxometalates. <i>Micro and Nano Letters</i> , 2014 , 9, 482-485	0.9	2
26	An applied quantum-chemical model for genipin-crosslinked chitosan (GCS) nanocarrier. <i>International Journal of Biological Macromolecules</i> , 2020 , 165, 1229-1240	7.9	2
25	Perception of the reciprocal influences of the formed interactions and hydrogen bonds, and adsorption energies between zinc-titanate nanoparticles/nano-silica/Dawson heteropolyacid hybrid- water on the positive alternation trends of the strength and properties of ordinary and self-compacting concrete: A systematic study through the quantum mechanical theory and experimental engineering studies. <i>Journal of Molecular Liquids</i> , 2021 , 326, 115518	6	2
24	Quantum chemical analysis of 5-aminolevulinic acid anticancer drug delivery systems: Carbon nanotube, COOH functionalized carbon nanotube and iron oxide nanoparticle. <i>Journal of Molecular Liquids</i> , 2021 , 340, 117182	6	2
23	A DFT study on the geometry, tautomerism and noncovalent interactions of the Mepivacaine drug with the pristine SWCNT and COOH functionalized SWCNT. <i>Journal of Theoretical and Computational Chemistry</i> , 2017 , 16, 1750008	1.8	1
22	Study of alpha-amylase and gold nanoparticles interaction at two different temperatures through molecular dynamics. <i>Journal of Molecular Graphics and Modelling</i> , 2019 , 88, 273-281	2.8	1
21	Computational Study of Regioselective Synthesis of Triflylpyrazole by Cycloaddition Reaction between Diphenyl Hydrazonoyl Chloride and Phenyl Triflyl Acetylene. <i>Russian Journal of Physical Chemistry A</i> , 2018 , 92, 271-279	0.7	1
20	A molecular dynamics study on the liquid SbCl5 and SbF5 using force fields derived from quantum chemical calculations. <i>Physics and Chemistry of Liquids</i> , 2013 , 51, 695-703	1.5	1
19	Synthesis, characterisation, optical properties and theoretical calculations of a new fluorescent heterocyclic system: 3H-benzo[a]pyrazolo[3,4-j]acridine. <i>Journal of Chemical Research</i> , 2017 , 41, 371-375	0.6	1
18	The computational study of the Fe2O3 nanoparticle as Carmustine drug delivery system: DFT approach		1
17	The scrutinised DFT and MD studies on the adsorption of D-penicillamine drug on Fe2O3 nanoparticle as a highly efficient carrier. <i>Molecular Simulation</i> , 2020 , 46, 408-418	2	1
16	Acetyl-11-keto-Eboswellic acid derivatives effects on 5-lipoxygenase: In silico viewpoint. <i>Journal of Molecular Graphics and Modelling</i> , 2020 , 94, 107464	2.8	1

15	Ultrasonic-assisted synthesis and structural characterization of a novel 3D Pb(II) metal-organic CPs and their nanostructures. <i>Inorganica Chimica Acta</i> , 2020 , 508, 119636	2.7	1
14	Synthesis, characterization, DFT and antibacterial studies of a novel vitamin B6 Schiff base and its Cu(II) and Zn(II) complexes. <i>Journal of Molecular Structure</i> , 2022 , 1248, 131452	3.4	1
13	Multivariate optimization of a novel potentiometric sensor to determine silver ions in real water and pharmacological product samples. <i>Monatshefte Für Chemie</i> , 2022 , 153, 227-235	1.4	1
12	Mechanistic, energetic and structural studies of carbon nanotubes functionalised with dihydroartemisinin drug in gas and solution phases. <i>Physics and Chemistry of Liquids</i> , 2018 , 56, 610-618	1.5	0
11	(E)-4-(((2-amino-5-chlorophenyl)imino)methyl)-5-(hydroxy-methyl)-2-methylpyridin-3-ol and its Cu(II) complex: Synthesis, DFT calculations and AIM analysis. <i>Journal of the Serbian Chemical Society</i> , 2020 , 85, 1033-1046	0.9	0
10	β-Cyclodextrin-lenalidomide anticancer drug delivery nanosystem: A quantum chemical approach. <i>Journal of Molecular Liquids</i> , 2021 , 344, 117762	6	0
9	Synthesis, characterization and in vitro evaluation of cytotoxicity and antibacterial properties of vanadyl complexes of the pyridoxal Schiff bases. <i>Journal of Molecular Structure</i> , 2021 , 1246, 131189	3.4	0
8	Mechanistic and energetic studies of superparamagnetic iron oxide nanoparticles as a cyclophosphamide anticancer drug nanocarrier: A quantum mechanical approach. <i>Progress in Reaction Kinetics and Mechanism</i> , 2019 , 44, 92-101	0.5	
7	Quantum mechanical investigation on the hydroxycarbonylation of styrene using a palladium complex catalyst. <i>Progress in Reaction Kinetics and Mechanism</i> , 2016 , 41, 215-223	0.5	
6	Geometry, tautomerism and non-covalent interactions of the drug halofuginone with the carbon-nanotube and Fe ₂ O ₃ nanoparticles: A DFT study. <i>Journal of the Serbian Chemical Society</i> , 2018 , 83, 305-315	0.9	
5	The Effect of Temperature on the Interaction of Phenanthroline-based Ligands with G-quadruplex: In Silico Viewpoint. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2019 , 22, 546-554	1.3	
4	Quantum-Chemical Modeling of Cyclic Peptide-Selenium Nanoparticle as an Anticancer Drug Nanocarrier. <i>Bulletin of the Korean Chemical Society</i> , 2020 , 41, 23-33	1.2	
3	Determination of Protonation Constants of Streptozocin in Different Aqueous Solutions of Methanol: Solvent Effect. <i>Russian Journal of Physical Chemistry A</i> , 2021 , 95, S71-S76	0.7	
2	Non-Covalent Hybridization of Carbon Nanotube by Single-Stranded DNA Homodecamers: in-silico Approach. <i>Russian Journal of Physical Chemistry A</i> , 2022 , 96, 145-151	0.7	
1	The New Antibacterial Agents Based on the Fused Aromatic Heterocyclic Compounds: Design, Synthesis, and Antibacterial Activity. <i>Russian Journal of General Chemistry</i> , 2022 , 92, 732-738	0.7	