Ali Morsali

List of Publications by Year in Descending Order

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	Synthesis, characterization, DFT and antibacterial studies of a novel vitamin B6 Schiff base and its Cu(II) and Zn(II) complexes. *Journal of Molecular Structure*, **2022**, 1248, 131452	3.4	1
85	Non-Covalent Hybridization of Carbon Nanotube by Single-Stranded DNA Homodecamers: in-silico Approach. *Russian Journal of Physical Chemistry A*, **2022**, 96, 145-151	0.7	
84	Multivariate optimization of a novel potentiometric sensor to determine silver ions in real water and pharmacological product samples. *Monatshefte F Chemie*, **2022**, 153, 227-235	1.4	1
83	The New Antibacterial Agents Based on the Fused Aromatic Heterocyclic Compounds: Design, Synthesis, and Antibacterial Activity. *Russian Journal of General Chemistry*, **2022**, 92, 732-738	0.7	
82	cyclodextrin-lenalidomide anticancer drug delivery nanosystem: A quantum chemical approach. *Journal of Molecular Liquids*, **2021**, 344, 117762	6	0
81	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	6	2
80	Determination of Protonation Constants of Streptozocin in Different Aqueous Solutions of Methanol: Solvent Effect. *Russian Journal of Physical Chemistry A*, **2021**, 95, S71-S76	0.7	
79	Green synthesis of zinc oxide and copper oxide nanoparticles using Achillea Nobilis extract and evaluating their antioxidant and antibacterial properties. *Bulletin of Materials Science*, **2021**, 44, 1	1.7	6
78	Quantum chemical analysis of 5-aminolevulinic acid anticancer drug delivery systems: Carbon nanotube, COOH functionalized carbon nanotube and iron oxide nanoparticle. *Journal of Molecular Liquids*, **2021**, 340, 117182	6	2
77	Synthesis, characterization and in vitro evaluation of cytotoxicity and antibacterial properties of vanadyl complexes of the pyridoxal Schiff bases. *Journal of Molecular Structure*, **2021**, 1246, 131189	3.4	0
76	Quantum molecular study of mesoporous silica nanoparticle as a delivery system for troxacitabine anticancer drug. *Journal of Molecular Liquids*, **2020**, 310, 113155	6	3
75	Synthesis, experimental and computational characterizations of a new quinoline derived Schiff base and its Mn(II), Ni(II) and Cu(II) complexes. *Journal of Molecular Structure*, **2020**, 1208, 127898	3.4	9
74	(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. *Journal of the Serbian Chemical Society*, **2020**, 85, 1033-1046	0.9	0
73	The scrutinised DFT and MD studies on the adsorption of D-penicillamine drug on Fe2O3 nanoparticle as a highly efficient carrier. *Molecular Simulation*, **2020**, 46, 408-418	2	1
72	Surface functionalization of chitosan with 5-nitroisatin. *International Journal of Biological Macromolecules*, **2020**, 147, 534-546	7.9	9
71	Quantum chemical studies of chitosan nanoparticles as effective drug delivery systems for 5-fluorouracil anticancer drug. *Journal of Molecular Liquids*, **2020**, 302, 112495	6	30
70	Quantum-Chemical Modeling of Cyclic Peptide-Selenium Nanoparticle as an Anticancer Drug Nanocarrier. *Bulletin of the Korean Chemical Society*, **2020**, 41, 23-33	1.2	

69	Stability appraisement of the alumina-brine nanofluid in the presence of ionic and non-ionic disparents on the alumina nanoparticles surface as heat transfer fluids: Quantum mechanical study and Taguchi-optimized experimental analysis. *Journal of Molecular Liquids*, **2020**, 319, 113898	6	7
68	An applied quantum-chemical model for genipin-crosslinked chitosan (GCS) nanocarrier. *International Journal of Biological Macromolecules*, **2020**, 165, 1229-1240	7.9	2
67	Density functional theory study towards investigating the adsorption properties of the Fe2O3 nanoparticles as a nanocarrier for delivery of Flutamide anticancer drug. *Adsorption*, **2020**, 26, 925-939	2.6	7
66	Acetyl-11-keto-boswellic acid derivatives effects on 5-lipoxygenase: In silico viewpoint. *Journal of Molecular Graphics and Modelling*, **2020**, 94, 107464	2.8	1
65	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. *Journal of Molecular Liquids*, **2020**, 297, 111912	6	5
64	Ultrasonic-assisted synthesis and structural characterization of a novel 3D Pb(II) metal-organic CPs and their nanostructures. *Inorganica Chimica Acta*, **2020**, 508, 119636	2.7	1
63	Mechanistic and energetic studies of superparamagnetic iron oxide nanoparticles as a cyclophosphamide anticancer drug nanocarrier: A quantum mechanical approach. *Progress in Reaction Kinetics and Mechanism*, **2019**, 44, 92-101	0.5	
62	Molecular mechanism study of surface functionalization of silica nanoparticle as an anticancer drug nanocarrier in aqueous solution. *Journal of Molecular Liquids*, **2019**, 282, 392-400	6	15
61	Quantum chemical modeling of iron oxide magnetic nanoparticles functionalized with cytarabine. *Chemical Physics Letters*, **2019**, 719, 12-21	2.5	9
60	Study of alpha-amylase and gold nanoparticles interaction at two different temperatures through molecular dynamics. *Journal of Molecular Graphics and Modelling*, **2019**, 88, 273-281	2.8	1
59	The Effect of Temperature on the Interaction of Phenanthroline-based Ligands with G-quadruplex: In Silico Viewpoint. *Combinatorial Chemistry and High Throughput Screening*, **2019**, 22, 546-554	1.3	
58	Role of repulsive forces on self-assembly behavior of amyloid peptide (1-40): Molecular dynamics simulation approach. *Physica A: Statistical Mechanics and Its Applications*, **2019**, 513, 524-535	3.3	3
57	Synthesis, experimental and theoretical characterizations of a 1,2,4-triazole Schiff base and its nickel(II) complex. *Journal of Molecular Structure*, **2019**, 1179, 779-786	3.4	11
56	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. *Journal of Molecular Graphics and Modelling*, **2019**, 86, 199-208	2.8	6
55	DFT study of SiO2 nanoparticles as a drug delivery system: structural and mechanistic aspects. *Structural Chemistry*, **2019**, 30, 715-726	1.8	12
54	The computational study of the FeO nanoparticle as Carmustine drug delivery system: DFT approach. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 454-464	3.6	19
53	Quantum Mechanical Study of Fe2O3 Nanoparticle as a Nanocarrier for Anticancer Drug Delivery. *Zeitschrift Fur Physikalische Chemie*, **2018**, 232, 579-592	3.1	6
52	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. *Journal of Molecular Graphics and Modelling*, **2018**, 80, 85-94	2.8	4

51	Computational Study of Regioselective Synthesis of Triflylpyrazole by Cycloaddition Reaction between Diphenyl Hydrazonoyl Chloride and Phenyl Triflyl Acetylene. *Russian Journal of Physical Chemistry A*, **2018**, 92, 271-279	0.7	1
50	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. *Applied Surface Science*, **2018**, 434, 492-503	6.7	57
49	Mechanistic, energetic and structural studies of carbon nanotubes functionalised with dihydroartemisinin drug in gas and solution phases. *Physics and Chemistry of Liquids*, **2018**, 56, 610-618	1.5	0
48	Treatment of the breast cancer by using low frequency electromagnetic fields and Mn(II) complex of a Schiff base derived from the pyridoxal. *Breast*, **2018**, 41, 107-112	3.6	12
47	Three VO2+ complexes of the pyridoxal-derived Schiff bases: Synthesis, experimental and theoretical characterizations, and catalytic activity in a cyclocondensation reaction. *Journal of Molecular Structure*, **2018**, 1153, 149-156	3.4	16
46	Comprehensive quantum chemical insight into the mechanistic understanding of the surface functionalization of carbon nanotube as a nanocarrier with cladribine anticancer drug. *Applied Surface Science*, **2018**, 462, 720-729	6.7	24
45	Geometry, tautomerism and non-covalent interactions of the drug halofuginone with the carbon-nanotube and □Fe2O3 nanoparticles: A DFT study. *Journal of the Serbian Chemical Society*, **2018**, 83, 305-315	0.9	
44	A DFT study on the geometry, tautomerism and noncovalent interactions of the Mepivacaine drug with the pristine SWCNT and □COOH functionalized SWCNT. *Journal of Theoretical and Computational Chemistry*, **2017**, 16, 1750008	1.8	1
43	Assessment of solvent effects on the interaction of Carmustine drug with the pristine and COOH-functionalized single-walled carbon nanotubes: A DFT perspective. *Journal of Molecular Liquids*, **2017**, 240, 87-97	6	31
42	Synthesis, experimental and theoretical characterizations of a new Schiff base derived from 2-pyridincarboxaldehyde and its Ni (II) complex. *Journal of Molecular Structure*, **2017**, 1143, 424-430	3.4	26
41	Synthesis, experimental and DFT characterization of the 2-((E)-(2-[(E)-2,3-Dihydroxybenzylideneamino]-5-methylphenyl)iminiomethyl)-6-hydroxyphenolate and its Ni(II) and Cu(II) complexes. *Journal of Molecular Structure*, **2017**, 1146, 620-628	3.4	6
40	Density Functional Theoretical Study on the Mechanism of Alcoholysis of Acylpalladium(II) Complexes. *Progress in Reaction Kinetics and Mechanism*, **2017**, 42, 52-61	0.5	2
39	Theoretical study of solvent and co-solvent effects on the interaction of Flutamide anticancer drug with Carbon nanotube as a drug delivery system. *Journal of Molecular Liquids*, **2017**, 248, 490-500	6	46
38	Quantum Mechanical Study on the Mechanistic, Energetic, and Structural Properties of Adsorption of 6-Thioguanine onto □Fe2O3 Nanoparticles. *Bulletin of the Korean Chemical Society*, **2017**, 38, 869-874	1.2	5
37	Synthesis, experimental and theoretical characterization of a Mn(II) complex of N,N?-dipyridoxyl(1,2-diaminobenzene). *Journal of Molecular Structure*, **2017**, 1127, 15-22	3.4	20
36	Kinetics and mechanism of producing 3,8-dimethyl-3H-imidazo[4,5-a]acridine-11-carbonitrile: a DFT investigation. *Research on Chemical Intermediates*, **2017**, 43, 1829-1846	2.8	2
35	Synthesis, characterisation, optical properties and theoretical calculations of a new fluorescent heterocyclic system: 3H-benzo[a]pyrazolo[3,4-j]acridine. *Journal of Chemical Research*, **2017**, 41, 371-375	0.6	1
34	Quantum mechanical investigation on the hydroxycarbonylation of styrene using a palladium complex catalyst. *Progress in Reaction Kinetics and Mechanism*, **2016**, 41, 215-223	0.5	

33	Theoretical Investigation on the Kinetics and Mechanism of the Synthesis of Fluorescent 3,8-Disubstituted-3H-Imidazo [4,5-a] Acridine-11-Carbonitriles. *Progress in Reaction Kinetics and Mechanism*, **2016**, 41, 365-370	0.5	8
32	Mechanism of the Formation of Palladium(II) Maleate Complex: A DFT Approach. *International Journal of Chemical Kinetics*, **2015**, 47, 73-81	1.4	13
31	A DFT investigation of structure, spectroscopic properties and tautomerism of the anticonvulsant drug Lyrica. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 138, 637-42	4.4	15
30	Extraordinary catalytic activity of a Keplerate-type giant nanoporous isopolyoxomolybdate in the synthesis of 1,8-dioxo-octahydroxanthenes and 1,8-dioxodecahydroacridines. *Research on Chemical Intermediates*, **2015**, 41, 7815-7826	2.8	17
29	QTAIM study of substituent effects on the intramolecular hydrogen bond in 3,3?-dihydroxy-4,4?-[5-methyl-1,3-phenylenebis(nitrilomethylidyne)]-bis-phenol. *Journal of Molecular Structure*, **2015**, 1083, 1-9	3.4	8
28	Quantum mechanical study of the alkoxide-independent pathway of reductive elimination of CO from palladium (p-cyanophenyl) neopentoxide complex. *Research on Chemical Intermediates*, **2015**, 41, 5389-5398	2.8	7
27	The study of self-aggregation behavior of the bilirubin molecules in the presence and absence of carbon nanotubes: Molecular dynamics simulation approach. *Journal of Molecular Liquids*, **2015**, 208, 342-346	6	5
26	Synthesis, characterization and intramolecular proton transfer of 3,3?-dihydroxy-4,4?-[5-methyl-1,3-phenylenebis(nitrilomethylidyne)]-bis-phenol. *Journal of Molecular Structure*, **2014**, 1072, 187-194	3.4	13
25	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. *Journal of Supercritical Fluids*, **2014**, 95, 628-634	4.2	2
24	Synthesis and characterisation of modified carbon nanotubes with potassium salts of the monosubstituted Keggin polyoxometalates. *Micro and Nano Letters*, **2014**, 9, 482-485	0.9	2
23	Theoretical and Experimental Studies on the Regioselectivity of Epoxide Ring Opening by Nucleophiles in Nitromethane without any Catalyst: Nucleophilic-Chain Attack Mechanism. *Progress in Reaction Kinetics and Mechanism*, **2014**, 39, 89-102	0.5	14
22	Quantum mechanical study on the mechanism and kinetics of the cis-to-trans isomerization of [Pd(C6Cl2F3)I(PH3)2]. *Inorganica Chimica Acta*, **2013**, 394, 423-429	2.7	16
21	Theoretical Study of Solvent Effects on the Cis-to-Trans Isomerization of [Pd(C6Cl2F3)I(PH3)2]. *Journal of Solution Chemistry*, **2013**, 42, 1902-1911	1.8	18
20	A molecular dynamics study on the liquid SbCl5 and SbF5 using force fields derived from quantum chemical calculations. *Physics and Chemistry of Liquids*, **2013**, 51, 695-703	1.5	1
19	A molecular dynamics study on the role of attractive and repulsive forces in excess heat capacity at constant volume of dense fluids. *Molecular Physics*, **2012**, 110, 483-490	1.7	3
18	Quantum mechanical study on the mechanism and kinetics of the hydrolysis of organopalladium Complex [Pd(CNN)P(OMe)3]+ in low acidity range. *Computational and Theoretical Chemistry*, **2012**, 994, 41-46	2	16
17	The changes in free energies and entropies from analytical radial distribution functions. *Physics and Chemistry of Liquids*, **2012**, 50, 187-198	1.5	4
16	N,NRdipyridoxyl Schiff bases: synthesis, experimental and theoretical characterization. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2011**, 83, 467-71	4.4	35

15	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. *Chinese Journal of Chemistry*, **2011**, 29, 1167-1172	4.9	3
14	S-allyl-3-(2-pyridyl-methylene)dithiocarbazate ligand and its manganese(II), cobalt(III) and nickel(II) complexes. *Inorganica Chimica Acta*, **2011**, 371, 36-41	2.7	37
13	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. *Bulletin of the Korean Chemical Society*, **2011**, 32, 1873-1878	1.2	8
12	The sound velocities in dense fluids from distribution functions. *Physics and Chemistry of Liquids*, **2010**, 48, 50-61	1.5	5
11	A density functional theory investigation of the bromide oxidation mechanism by a vanadium bromoperoxidase model complex. *Transition Metal Chemistry*, **2010**, 35, 939-947	2.1	4
10	OH bond cleavage step of the Wacker process: A DFT study. *Computational and Theoretical Chemistry*, **2010**, 941, 138-143		17
9	THE HEAT CAPACITIES FROM ANALYTICAL DISTRIBUTION FUNCTIONS. *Journal of Theoretical and Computational Chemistry*, **2009**, 08, 943-956	1.8	4
8	H-Transfer steps of the Wacker process: A DFT study. *Computational and Theoretical Chemistry*, **2009**, 903, 108-114		29
7	Mechanism and Kinetics of the Wacker Process: A Quantum Mechanical Approach. *Organometallics*, **2008**, 27, 72-79	3.8	56
6	Synthesis, experimental and theoretical characterization of tetra dentate N,NRdipyridoxyl (1,3-propylenediamine) salen ligand and its Co(III) complex. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2008**, 71, 1341-7	4.4	37
5	A molecular dynamics study on the role of attractive and repulsive forces in internal energy, internal pressure and structure of dense fluids. *Chemical Physics*, **2007**, 331, 332-338	2.3	15
4	Evaluation of PVT differential properties of the Lennard-Jones fluid using radial distribution functions and molecular dynamics. *Chemical Physics*, **2007**, 335, 194-200	2.3	9
3	An accurate expression for radial distribution function of the Lennard-Jones fluid. *Chemical Physics*, **2005**, 310, 11-15	2.3	36
2	New regularities and an equation of state for liquids. *Fluid Phase Equilibria*, **2005**, 230, 170-175	2.5	60
1	The computational study of the Fe2O3 nanoparticle as Carmustine drug delivery system: DFT approach		1