# Ali Morsali

List of Publications by Year
in descending order



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|---|---|---|---|
| 86 papers | 1,245 citations | 361045 20 h-index | 433756 31 g-index |
| 87 all docs | 87 docs citations | 87 times ranked | 903 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | 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. | 3.1 | 87 |
| 2 | New regularities and an equation of state for liquids. Fluid Phase Equilibria, 2005, 230, 170-175. | 1.4 | 64 |
| 3 | 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. | 2.3 | 60 |
| 4 | Mechanism and Kinetics of the Wacker Process: A Quantum Mechanical Approach. Organometallics, 2008, 27, 72-79. | 1.1 | 58 |
| 5 | 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. | 2.3 | 52 |
| 6 | An accurate expression for radial distribution function of the Lennard-Jones fluid. Chemical Physics, 2005, 310, 11-15. | 0.9 | 44 |
| 7 | 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. | 1.2 | 43 |
| 8 | Quantum chemical studies of chitosan nanoparticles as effective drug delivery systems for 5-fluorouracil anticancer drug. Journal of Molecular Liquids, 2020, 302, 112495. | 2.3 | 43 |
| 9 | Synthesis, experimental and theoretical characterization of tetra dentate N,Nâ€²-dipyridoxyl (1,3-propylenediamine) salen ligand and its Co(III) complex. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 1341-1347. | 2.0 | 41 |
| 10 | N,Nâ€²-dipyridoxyl Schiff bases: Synthesis, experimental and theoretical characterization. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 83, 467-471. | 2.0 | 41 |
| 11 | 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. | 3.1 | 34 |
| 12 | H-Transfer steps of the Wacker process: A DFT study. Computational and Theoretical Chemistry, 2009, 903, 108-114. | 1.5 | 31 |
| 13 | 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. | 1.8 | 31 |
| 14 | Three VO 2+ 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. | 1.8 | 29 |
| 15 | The computational study of the Î³-Fe<sub>2</sub>O<sub>3</sub> nanoparticle as Carmustine drug delivery system: DFT approach. Journal of Biomolecular Structure and Dynamics, 2019, 37, 454-464. | 2.0 | 28 |
| 16 | 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. | 1.8 | 25 |
| 17 | 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. | 0.8 | 24 |
| 18 | Synthesis, experimental and theoretical characterization of a Mn(II) complex of N,Nâ€²-dipyridoxyl(1,2-diaminobenzene). Journal of Molecular Structure, 2017, 1127, 15-22. | 1.8 | 23 |

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|---|---|---|---|
| 19 | DFT study of SiO2 nanoparticles as a drug delivery system: structural and mechanistic aspects. Structural Chemistry, 2019, 30, 715-726. | 1.0 | 21 |
| 20 | 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. | 1.3 | 20 |
| 21 | 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. | 2.3 | 20 |
| 22 | 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. | 0.6 | 18 |
| 23 | 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. | 0.9 | 18 |
| 24 | OH bond cleavage step of the Wacker process: A DFT study. Computational and Theoretical Chemistry, 2010, 941, 138-143. | 1.5 | 17 |
| 25 | 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. | 1.8 | 17 |
| 26 | 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. | 1.1 | 16 |
| 27 | 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. | 1.2 | 16 |
| 28 | 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. | 0.9 | 15 |
| 29 | 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. | 1.1 | 15 |
| 30 | A DFT investigation of structure, spectroscopic properties and tautomerism of the anticonvulsant drug Lyrica. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 138, 637-642. | 2.0 | 15 |
| 31 | Quantum chemical analysis of 5-aminolevulinic acid anticancer drug delivery systems: Carbon nanotube, â€“COOH functionalized carbon nanotube and iron oxide nanoparticle. Journal of Molecular Liquids, 2021, 340, 117182. | 2.3 | 14 |
| 32 | Synthesis, characterization and intramolecular proton transfer of 3,3â€²-dihydroxy-4,4â€²-[5-methyl-1,3-phenylenebis(nitrilomethylidyne)]-bis-phenol. Journal of Molecular Structure, 2014, 1072, 187-194. | 1.8 | 13 |
| 33 | Mechanism of the Formation of Palladium(II) Maleate Complex: A DFT Approach. International Journal of Chemical Kinetics, 2015, 47, 73-81. | 1.0 | 13 |
| 34 | Density functional theory study towards investigating the adsorption properties of the Î³-Fe2O3 nanoparticles as a nanocarrier for delivery of Flutamide anticancer drug. Adsorption, 2020, 26, 925-939. | 1.4 | 12 |
| 35 | Surface functionalization of chitosan with 5-nitroisatin. International Journal of Biological Macromolecules, 2020, 147, 534-546. | 3.6 | 12 |
| 36 | An applied quantum-chemical model for genipin-crosslinked chitosan (GCS) nanocarrier. International Journal of Biological Macromolecules, 2020, 165, 1229-1240. | 3.6 | 12 |

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|---|---|---|---|
| 37 | Quantum chemical modeling of iron oxide magnetic nanoparticles functionalized with cytarabine. Chemical Physics Letters, 2019, 719, 12-21. | 1.2 | 11 |
| 38 | 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. | 1.3 | 11 |
| 39 | Evaluation of Pâ€“Vâ€“T differential properties of the Lennard-Jones fluid using radial distribution functions and molecular dynamics. Chemical Physics, 2007, 335, 194-200. | 0.9 | 10 |
| 40 | 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. | 1.1 | 9 |
| 41 | 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. | 1.0 | 9 |
| 42 | The sound velocities in dense fluids from distribution functions. Physics and Chemistry of Liquids, 2010, 48, 50-61. | 0.4 | 8 |
| 43 | QTAIM study of substituent effects on the intramolecular hydrogen bond in 3,3â€²-dihydroxy-4,4â€²-[5-methyl-1,3-phenylenebis(nitrilomethylidyne)]-bis-phenol. Journal of Molecular Structure, 2015, 1083, 1-9. | 1.8 | 8 |
| 44 | Quantum mechanical study of the alkoxide-independent pathway of reductive elimination of Câ€“O from palladium (p-cyanophenyl) neopentoxide complex. Research on Chemical Intermediates, 2015, 41, 5389-5398. | 1.3 | 8 |
| 45 | 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. | 2.3 | 8 |
| 46 | Quantum molecular study of mesoporous silica nanoparticle as a delivery system for troxacitabine anticancer drug. Journal of Molecular Liquids, 2020, 310, 113155. | 2.3 | 8 |
| 47 | 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. | 2.3 | 7 |
| 48 | 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. | 1.8 | 7 |
| 49 | Role of repulsive forces on self-assembly behavior of amyloid<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll" id="d1e748" altimg="si46.gif"><mml:mi>Î²</mml:mi></mml:math>-peptide (1-40): Molecular dynamics simulation approach. Physica A: Statistical Mechanics and Its Applications, 2019, 513, 524-535. | 1.2 | 7 |
| 50 | Quantum Mechanical Study of Î³-Fe<sub>2</sub>O<sub>3</sub> Nanoparticle as a Nanocarrier for Anticancer Drug Delivery. Zeitschrift Fur Physikalische Chemie, 2018, 232, 579-592. | 1.4 | 6 |
| 51 | 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. | 2.3 | 6 |
| 52 | 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. | 1.8 | 6 |
| 53 | A density functional theory investigation of the bromide oxidation mechanism by a vanadium bromoperoxidase model complex. Transition Metal Chemistry, 2010, 35, 939-947. | 0.7 | 5 |
| 54 | The changes in free energies and entropies from analytical radial distribution functions. Physics and Chemistry of Liquids, 2012, 50, 187-198. | 0.4 | 5 |

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|---|---|---|---|
| 55 | Quantum Mechanical Study on the Mechanistic, Energetic, and Structural Properties of Adsorption of 6â€Thioguanine onto Î³â€<scp>Fe<sub>2</sub>O<sub>3</sub></scp> Nanoparticles. Bulletin of the Korean Chemical Society, 2017, 38, 869-874. | 1.0 | 5 |
| 56 | Does high pressure have any effect on the structure of alpha amylase and its ability to binding to the oligosaccharides having 3â€“7 residues? Molecular dynamics study. Journal of Molecular Graphics and Modelling, 2018, 80, 85-94. | 1.3 | 5 |
| 57 | Î²-cyclodextrin-lenalidomide anticancer drug delivery nanosystem: A quantum chemical approach. Journal of Molecular Liquids, 2021, 344, 117762. | 2.3 | 5 |
| 58 | THE HEAT CAPACITIES FROM ANALYTICAL DISTRIBUTION FUNCTIONS. Journal of Theoretical and Computational Chemistry, 2009, 08, 943-956. | 1.8 | 4 |
| 59 | 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. | 1.3 | 4 |
| 60 | Ultrasonic-assisted synthesis and structural characterization of a novel 3D Pb(II) metal-organic CPs and their nanostructures. Inorganica Chimica Acta, 2020, 508, 119636. | 1.2 | 4 |
| 61 | 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. | 2.6 | 3 |
| 62 | 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. | 0.8 | 3 |
| 63 | 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. | 0.4 | 3 |
| 64 | 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. | 1.8 | 3 |
| 65 | Multivariate optimization of a novel potentiometric sensor to determine silver ions in real water and pharmacological product samples. Monatshefte FÃ¼r Chemie, 2022, 153, 227-235. | 0.9 | 3 |
| 66 | 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. | 1.6 | 2 |
| 67 | Synthesis and characterisation of modified carbon nanotubes with potassium salts of the monosubstituted Keggin polyoxometalates. Micro and Nano Letters, 2014, 9, 482-485. | 0.6 | 2 |
| 68 | Density Functional Theoretical Study on the Mechanism of Alcoholysis of Acylpalladium(II) Complexes. Progress in Reaction Kinetics and Mechanism, 2017, 42, 52-61. | 1.1 | 2 |
| 69 | 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. | 1.3 | 2 |
| 70 | Acetyl-11-keto-Î²-boswellic acid derivatives effects on 5-lipoxygenase: In silico viewpoint. Journal of Molecular Graphics and Modelling, 2020, 94, 107464. | 1.3 | 2 |
| 71 | 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. Journal of Molecular Liquids, 2021, 326, 115318. | 2.3 | 2 |
| 72 | A molecular dynamics study on the liquid SbCl5and SbF5using force fields derived from quantum chemical calculations. Physics and Chemistry of Liquids, 2013, 51, 695-703. | 0.4 | 1 |

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|---|---|---|---|
| 73 | Quantum mechanical investigation on the hydroxycarbonylation of styrene using a palladium complex catalyst. Progress in Reaction Kinetics and Mechanism, 2016, 41, 215-223. | 1.1 | 1 |
| 74 | A DFT study on the geometry, tautomerism and noncovalent interactions of the Mepivacaine drug with the pristine SWCNT and â€“COOH functionalized SWCNT. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750008. | 1.8 | 1 |
| 75 | 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 |
| 76 | 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. | 0.1 | 1 |
| 77 | The computational study of the Î³-Fe2O3 nanoparticle as Carmustine drug delivery system: DFT approach. , 0, . | | 1 |
| 78 | The scrutinised DFT and MD studies on the adsorption of D-penicillamine drug on Î³-Fe<sub>2</sub>O<sub>3</sub> nanoparticle as a highly efficient carrier. Molecular Simulation, 2020, 46, 408-418. | 0.9 | 1 |
| 79 | (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. | 0.4 | 1 |
| 80 | 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. | 0.3 | 1 |
| 81 | 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. | 1.1 | 0 |
| 82 | Quantumâ€Chemical Modeling of Cyclic Peptideâ€Selenium Nanoparticle as an Anticancer Drug Nanocarrier. Bulletin of the Korean Chemical Society, 2020, 41, 23-33. | 1.0 | 0 |
| 83 | Determination of Protonation Constants of Streptozocin in Different Aqueous Solutions of Methanol: Solvent Effect. Russian Journal of Physical Chemistry A, 2021, 95, S71-S76. | 0.1 | 0 |
| 84 | Geometry, tautomerism and non-covalent interactions of the drug halofuginone with the carbon-nanotube and Î³-Fe2O3 nanoparticles: A DFT study. Journal of the Serbian Chemical Society, 2018, 83, 305-315. | 0.4 | 0 |
| 85 | 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. | 0.6 | 0 |
| 86 | Non-Covalent Hybridization of Carbon Nanotube by Single-Stranded DNA Homodecamers: in-silico Approach. Russian Journal of Physical Chemistry A, 2022, 96, 145-151. | 0.1 | 0 |