# Majid Monajjemi

## List of Publications by Citations



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| 225 papers | 1,800 citations | 21 h-index | 32 g-index |
| 267 ext. papers | 1,988 ext. citations | 1.4 avg, IF | 5.19 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 225 | The Studies of Equilibrium and Thermodynamic Adsorption of Pb(II), Cd(II) and Cu(II) Ions from Aqueous Solution onto SWCNTs and SWCNT-COOH Surfaces. *Fullerenes Nanotubes and Carbon Nanostructures*, **2010**, 18, 285-302 | 1.8 | 110 |
| 224 | The study of adsorption characteristics Cu2+ and Pb2+ ions onto PHEMA and P(MMA-HEMA) surfaces from aqueous single solution. *Journal of Hazardous Materials*, **2009**, 170, 673-9 | 12.8 | 110 |
| 223 | Efficient removal of toxic bromothymol blue and methylene blue from wastewater by polyvinyl alcohol. *Journal of Molecular Liquids*, **2016**, 218, 191-197 | 6 | 109 |
| 222 | Theoretical Description of Electromagnetic Nonbonded Interactions of Radical, Cationic, and Anionic NH2BHNBHNH2 Inside of the B18N18 Nanoring. *Journal of Physical Chemistry C*, **2010**, 114, 15315-15330 | 3.8 | 45 |
| 221 | Theoretical investigation of hydrogen bonding in Watson-Crick, Hoogestein and their reversed and other models: comparison and analysis for configurations of adenine-thymine base pairs in 9 models. *Computational and Theoretical Chemistry*, **2005**, 714, 43-60 | | 38 |
| 220 | Quantum investigation of non-bonded interaction between the B15N15 ring and BH2NBH2 (radical, cation, anion) systems: a nano molecularmotor. *Structural Chemistry*, **2012**, 23, 551-580 | 1.8 | 35 |
| 219 | Synthesis of nanocomposites of iron oxide/gold (FeO/Au) loaded on activated carbon and their application in water treatment by using sonochemistry: Optimization study. *Ultrasonics Sonochemistry*, **2018**, 41, 279-287 | 8.9 | 33 |
| 218 | A new generation of B(n)N(n) rings as a supplement to boron nitride tubes and cages. *Journal of Physical Chemistry A*, **2013**, 117, 1670-84 | 2.8 | 30 |
| 217 | Liquid-phase exfoliation (LPE) of graphite towards graphene: An ab initio study. *Journal of Molecular Liquids*, **2017**, 230, 461-472 | 6 | 29 |
| 216 | Molecular Modeling Study of Drug-DNA Combined to Single Walled Carbon Nanotube. *Journal of Cluster Science*, **2012**, 23, 259-272 | 3 | 28 |
| 215 | Non bonded interaction between BnNn (stator) and (rotor) systems: A quantum rotation in IR region. *Chemical Physics*, **2013**, 425, 29-45 | 2.3 | 27 |
| 214 | Computational investigation on alcohol nanosensors in combination with carbon nanotube: a Monte Carlo and ab initio simulation. *Ionics*, **2013**, 19, 155-164 | 2.7 | 27 |
| 213 | EPR Study of Electronic Structure of [CoF6]3- and B18N18 Nano Ring Field Effects on Octahedral Complex. *Journal of Cluster Science*, **2011**, 22, 673-692 | 3 | 26 |
| 212 | Theoretical Studies of Solvent Effect on Normal Mode Analysis and Thermodynamic Properties of Zigzag (5, 0) Carbon Nanotube. *Fullerenes Nanotubes and Carbon Nanostructures*, **2011**, 19, 469-482 | 1.8 | 26 |
| 211 | NMR contour maps as a new parameter of carboxyl- OH groups in amino acids recognition: A reason of tRNA-amino acid conjugation. *Chemical Physics*, **2014**, 433, 1-11 | 2.3 | 24 |
| 210 | Comparison of 4-chloro-2-nitrophenol adsorption on single-walled and multi-walled carbon nanotubes. *Iranian Journal of Environmental Health Science & Engineering*, **2012**, 9, 5 | | 24 |
| 209 | Solvent effects on relative stabilities and 14N NMR shielding of cytosine tautomers: continuous set of gauge transformation calculation using polarizable continuum model. *Computational and Theoretical Chemistry*, **2002**, 581, 51-58 | | 23 |

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| 208 | Solvent dielectric effect and side chain mutation on the structural stability of Burkholderia cepacia lipase active site: a quantum mechanical/molecular mechanics study. *Acta Biotheoretica*, **2011**, 59, 291-312 | 1.1 | 22 |
| 207 | NQR and NMR study of hydrogen bonding interactions in anhydrous and monohydrated guanine cluster model: A computational study. *Journal of Structural Chemistry*, **2009**, 50, 67-77 | 0.9 | 22 |
| 206 | Interaction of Na, Mg, Al, Si with carbon nanotube (CNT): NMR and IR study. *Russian Journal of Inorganic Chemistry*, **2009**, 54, 1465-1473 | 1.5 | 22 |
| 205 | The effects of mono- and divalent metal cations on the solution structure of caffeine and theophylline. *Journal of Molecular Structure*, **2004**, 705, 35-39 | 3.4 | 21 |
| 204 | Tin(II)-selective membrane potentiometric sensor using a crown ether as neutral carrier. *Sensors and Actuators B: Chemical*, **2005**, 107, 756-761 | 8.5 | 21 |
| 203 | Ionic Strength Dependence of Formation Constants: Complexation of Mo(VI) with Aspartic Acid. *Journal of Chemical & Engineering Data*, **2001**, 46, 1140-1144 | 2.8 | 20 |
| 202 | The pseudo JahnTeller effect of puckering in pentatomic unsaturated rings C4AE5, A = N, P, As, E = H, F, Cl. *Computational and Theoretical Chemistry*, **2015**, 1074, 19-25 | 2 | 19 |
| 201 | DFT outlook of solvent effect on function of nano bioorganic drugs. *Physics and Chemistry of Liquids* , **2012**, 50, 596-604 | 1.5 | 19 |
| 200 | Simulation of DNA bases in water: Comparison of the Monte Carlo algorithm with molecular mechanics force fields. *Biochemistry (Moscow)*, **2006**, 71 Suppl 1, S1-8 | 2.9 | 19 |
| 199 | A percolation model for carbon nanotube-polymer composites using the Mandelbrot-Given curve. *Journal of Structural Chemistry*, **2011**, 52, 54-59 | 0.9 | 18 |
| 198 | Theoretical Investigation of Carbon Nanotube Binding to DNA in View of Drug Delivery. *Journal of Computational and Theoretical Nanoscience*, **2011**, 8, 1212-1219 | 0.3 | 17 |
| 197 | Investigation of NMR shielding tensors in 1,3 dipolar cycloadditions: solvents dielectric effect. *Physics and Chemistry of Liquids*, **2008**, 46, 299-306 | 1.5 | 17 |
| 196 | Alcohol sensors based on SWNT as chemical sensors: Monte Carlo and Langevin dynamics simulation. *Microelectronics Journal*, **2010**, 41, 142-149 | 1.8 | 16 |
| 195 | Metal-doped graphene layers composed with boron nitride-graphene as an insulator: a nano-capacitor. *Journal of Molecular Modeling*, **2014**, 20, 2507 | 2 | 15 |
| 194 | Investigation of different factors towards synthesis of CuS spherical nanoparticles. *Journal of Experimental Nanoscience*, **2013**, 8, 451-461 | 1.9 | 15 |
| 193 | Exchange and Correlation Effect of Hydrogen Chemisorption on Nano V(100) Surface: A DFT Study by Generalized Gradient Approximation (GGA). *Journal of Computational and Theoretical Nanoscience*, **2011**, 8, 763-768 | 0.3 | 15 |
| 192 | Theoretical study of solvent effect on NMR shielding tensors of luciferin derivatives. *Physics and Chemistry of Liquids*, **2011**, 49, 561-571 | 1.5 | 15 |
| 191 | Thermodynamic investigation of the ternary mixed electrolyte (CoCl2 + CoSO4 + H2O) system by EMF measurements at T = 298.15 K. *Journal of Chemical Thermodynamics*, **2010**, 42, 1494-1499 | 2.9 | 15 |

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| 190 | Metal-stabilized rare tautomers: N4 metalated cytosine (M = Li+, Na+, K+, Rb+ and Cs+), theoretical views. *Applied Organometallic Chemistry*, **2003**, 17, 635-640 | 3.1 | 15 |
| 189 | Monte Carlo Quantum Calculation for Double-Walled Carbon Nanotubes (DWNTs) Combined to Calixarene[6]. *Journal of Computational and Theoretical Nanoscience*, **2013**, 10, 2332-2341 | 0.3 | 14 |
| 188 | Ab initio Study of Direct Diffusion Pathway for H+, Li+, Na+, K+ Cations into the (3,3), (4,4), and (5,5) Open-Ended Single-Walled Carbon Nanotubes. *Fullerenes Nanotubes and Carbon Nanostructures*, **2012**, 20, 163-169 | 1.8 | 14 |
| 187 | Theoretical Study of Different Solvent and Temperature Effects on Double-walled Carbon Nanotubes (DWNTs) and Calixarene with Amino Acid: A QM/MM Study. *Fullerenes Nanotubes and Carbon Nanostructures*, **2014**, 22, 346-361 | 1.8 | 13 |
| 186 | Carbon Nanotube as a Deliver for Sulforaphane in Broccoli Vegetable in Point of Nuclear Magnetic Resonance and Natural Bond Orbital Specifications. *Journal of Computational and Theoretical Nanoscience*, **2014**, 11, 1465-1471 | 0.3 | 13 |
| 185 | Molecular Modeling Investigation of an Anti-cancer Agent Joint to SWCNT Using Theoretical Methods. *Fullerenes Nanotubes and Carbon Nanostructures*, **2014**, 22, 738-751 | 1.8 | 13 |
| 184 | Thermodynamic study of solvent effects on nanostructures: phosphatidylserine and phosphatidylinositol membranes. *Physics and Chemistry of Liquids*, **2012**, 50, 161-172 | 1.5 | 13 |
| 183 | Theoretical Study of Boron Nitride Nanotubes with Armchair Forms. *Fullerenes Nanotubes and Carbon Nanostructures*, **2013**, 21, 381-393 | 1.8 | 12 |
| 182 | Dielectric effect on thermodynamic properties in vinblastine by DFT/Onsager modelling. *Physics and Chemistry of Liquids*, **2011**, 49, 318-336 | 1.5 | 12 |
| 181 | Interaction between threonine and cadmium cation in [Cd(Thr) n ]2+ (n = 1□) complexes: density functional calculations. *Russian Chemical Bulletin*, **2010**, 59, 886-889 | 1.7 | 12 |
| 180 | Electron transport phenomenon simulation through the carborane nano-molecular wire. *Physica E: Low-Dimensional Systems and Nanostructures*, **2008**, 40, 2965-2972 | 3 | 12 |
| 179 | Monte Carlo simulation study of melittin: Protein folding and temperature dependence. *Russian Journal of Physical Chemistry A*, **2006**, 80, S55-S62 | 0.7 | 12 |
| 178 | Preparation and characterization of Chicory leaf powder and its application as a nano-native plant sorbent for removal of Acid Blue 25 from aqueous media: isotherm, kinetic and thermodynamic study of the adsorption phenomenon. *Journal of Nanostructure in Chemistry*, **2020**, 10, 75-86 | 7.6 | 11 |
| 177 | Amino Functionalized Nano Fe3O4@SiO2 as a Magnetically Green Catalyst for the One-Pot Synthesis of Spirooxindoles Under Mild Conditions. *Polycyclic Aromatic Compounds*, **2018**, 38, 199-212 | 1.3 | 11 |
| 176 | Theoretical Study of Different Solvents and Temperatures Effects on Single-Walled Carbon Nanotube and Temozolomide Drug: A QM/MM Study. *Fullerenes Nanotubes and Carbon Nanostructures*, **2011**, 19, 653-667 | 1.8 | 11 |
| 175 | Substituent and solvent effects on the structural bioactivity and anticancer characteristic of catechin as a bioactive constituent of green tea. *International Journal of Quantum Chemistry*, **2011**, 111, 2771-2777 | 2.1 | 11 |
| 174 | Thermodynamic Investigation of Enol<-Keto Tautomerism for Alcohol Sensors Based on Carbon Nanotubes as Chemical Sensors. *Fullerenes Nanotubes and Carbon Nanostructures*, **2010**, 18, 45-55 | 1.8 | 11 |
| 173 | Design of fMet-tRNA and calculation of its bonding properties by quantum mechanics. *Nucleosides, Nucleotides and Nucleic Acids*, **2010**, 29, 676-83 | 1.4 | 11 |

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| 172 | Investigation of single wall carbon nanotubes electrical properties and normal mode analysis: Dielectric effects. *Russian Journal of Physical Chemistry A*, **2009**, 83, 2288-2296 | 0.7 | 11 |
| 171 | Intermolecular Simulation of Nanobiological Structures in Point of Potential Energy and Second Virial Coefficient. *Journal of Computational and Theoretical Nanoscience*, **2012**, 9, 2208-2214 | 0.3 | 11 |
| 170 | Interaction of Tl+3 with mononucleotides: metal ion binding and sugar conformation. *Journal of Molecular Structure*, **2001**, 562, 35-43 | 3.4 | 11 |
| 169 | Non-covalent attraction of B2N(Ⅰ) and repulsion of B2N(+) in the B n N n ring: a quantum rotatory due to an external field. *Theoretical Chemistry Accounts*, **2015**, 134, 1 | 1.9 | 10 |
| 168 | Vibrational analysis of p - tert -butyl-calix[4]arene conformers by ab initio calculations. *Physics and Chemistry of Liquids*, **2008**, 46, 379-389 | 1.5 | 10 |
| 167 | Study of the hydrogen bond in different orientations of adenine-thymine base pairs: an ab initio study. *Biochemistry (Moscow)*, **2005**, 70, 366-76 | 2.9 | 10 |
| 166 | Combined 3D-QSAR modeling and molecular docking study on multi-acting quinazoline derivatives as HER2 kinase inhibitors. *EXCLI Journal*, **2013**, 12, 130-43 | 2.4 | 10 |
| 165 | Nano Theoretical Study of a C16 Cluster as a Novel Material for Vitamin C Carrier. *Fullerenes Nanotubes and Carbon Nanostructures*, **2014**, 22, 687-708 | 1.8 | 9 |
| 164 | Sensor Response to Alcohol and Chemical Mechanism of Carbon Nanotube Gas Sensors. *Fullerenes Nanotubes and Carbon Nanostructures*, **2009**, 17, 484-495 | 1.8 | 9 |
| 163 | Quantum mechanic study of hydrogen chemisorptions on nanocluster vanadium surface. *Russian Journal of Inorganic Chemistry*, **2008**, 53, 1430-1437 | 1.5 | 9 |
| 162 | Complexation behaviour of p-t -butyl-calix[4]arene propoxy derivatives toward alkali metal cations in chloroform. *Physics and Chemistry of Liquids*, **2006**, 44, 449-456 | 1.5 | 9 |
| 161 | S-NICS: An Aromaticity Criterion for Nano Molecules. *Journal of Computational and Theoretical Nanoscience*, **2015**, 12, 4895-4914 | 0.3 | 9 |
| 160 | Density Functional Theory Study on B30N20 Nanocage in Structural Properties and Thermochemical Outlook. *Fullerenes Nanotubes and Carbon Nanostructures*, **2013**, 21, 503-515 | 1.8 | 8 |
| 159 | (3,3)4 Armchair Carbon Nanotube in Connection with PNP and NPN Junctions: Ab Initio and DFT-Based Studies. *Fullerenes Nanotubes and Carbon Nanostructures*, **2013**, 21, 213-232 | 1.8 | 8 |
| 158 | THE EFFECT OF DIFFERENT SOLVENTS AND TEMPERATURES ON STABILITY OF SINGLE-WALLED CARBON NANOTUBE: A QM/MD STUDY. *International Journal of Nanoscience*, **2010**, 09, 517-529 | 0.6 | 8 |
| 157 | Investigation of Solvent Effects on Armchair Single-Walled Carbon Nanotubes: A QM/MD Study. *Fullerenes Nanotubes and Carbon Nanostructures*, **2011**, 19, 251-261 | 1.8 | 8 |
| 156 | Thermodynamic study of interaction of TSPP, CoTsPc, and FeTsPc with calf thymus DNA. *Biochemistry (Moscow)*, **2007**, 72, 652-7 | 2.9 | 8 |
| 155 | A theoretical thermochemical study of solute-solvent dielectric effects in the displacement of codon-anticodon base pairs. *Russian Journal of Physical Chemistry A*, **2008**, 82, 2277-2285 | 0.7 | 8 |

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| 154 | Theoretical study of borthiin and its derivatives: structure and aromaticity. *Journal of Sulfur Chemistry*, **2007**, 28, 505-511 | 2.3 | 8 |
| 153 | Thermodynamic Studies on Complexation of Glutamic Acid with Dioxovanadium(V) in Mixed Solvent Systems. *Journal of Chemical & Engineering Data*, **2001**, 46, 1249-1254 | 2.8 | 8 |
| 152 | Cell membrane causes the lipid bilayers to behave as variable capacitors: A resonance with self-induction of helical proteins. *Biophysical Chemistry*, **2015**, 207, 114-27 | 3.5 | 7 |
| 151 | The Investigation of Sequence-dependent Interaction of Messenger RNA Binding to Carbon Nanotube. *Fullerenes Nanotubes and Carbon Nanostructures*, **2014**, 22, 643-662 | 1.8 | 7 |
| 150 | Non Bonded Interaction of B16N16 Nano Ring with Copper Cations in Point of Crystal Fields. *Journal of Computational and Theoretical Nanoscience*, **2013**, 10, 2473-2477 | 0.3 | 7 |
| 149 | Determination of thermodynamic properties of aqueous mixtures of MgCl2 and Mg(NO3)2 by the potentiometric method at T=298.15. *Fluid Phase Equilibria*, **2011**, 301, 98-104 | 2.5 | 7 |
| 148 | DFT study of metal□etrahydroborato ligand interactions in [Ti(CO)4(BH4)]□*Computational and Theoretical Chemistry*, **2003**, 625, 305-314 | | 7 |
| 147 | AB INITIO STUDY OF THE INTERACTION OF GUANINE, ADENINE, THYMINE AND CYTOSINE WITH Li+, Na+, Mg2+ AND Sr2+. *Main Group Metal Chemistry*, **2002**, 25, | 1.6 | 7 |
| 146 | Role of the salt bridge between Arg176 and Glu126 in the thermal stability of the Bacillus amyloliquefaciens □amylase (BAA). *Journal of Microbiology and Biotechnology*, **2013**, 23, 7-14 | 3.3 | 7 |
| 145 | Charge Density Discrepancy Between NBO and QTAIM in Single-wall Armchair Carbon Nanotubes. *Fullerenes Nanotubes and Carbon Nanostructures*, **2014**, 22, 575-594 | 1.8 | 6 |
| 144 | Thermochemistry and NBO analysis of peptide bond: Investigation of basis sets and binding energy. *Russian Journal of Physical Chemistry A*, **2009**, 83, 587-597 | 0.7 | 6 |
| 143 | Fractal Dimension on Carbon Nanotube-Polymer Composite Materials Using Percolation Theory. *Journal of Computational and Theoretical Nanoscience*, **2012**, 9, 597-601 | 0.3 | 6 |
| 142 | A DFT study of hydrogen chemisorption on V (100) surfaces. *Russian Journal of Physical Chemistry A*, **2008**, 82, 2354-2361 | 0.7 | 6 |
| 141 | Theoretical studies of rotational barriers of dithiocarbamate ligands in the square planar complexes TM(L)(L?)(H2dtc) (TM=Ir, Rh). *Computational and Theoretical Chemistry*, **2003**, 636, 49-56 | | 6 |
| 140 | Interaction of Nano-Boron Nitride/Graphene Sheets with Anode Lithium Ion Battery. *Journal of Computational and Theoretical Nanoscience*, **2016**, 13, 3070-3082 | 0.3 | 6 |
| 139 | Graphene/(h-BN) n/X-doped graphene as anode material in lithium ion batteries (X=Li, Be, B and N). *Macedonian Journal of Chemistry and Chemical Engineering*, **2017**, 36, 101 | 1.1 | 6 |
| 138 | Preparation and characterization of vancomycin-loaded chitosan/PVA/PEG hydrogels for wound dressing. *Materials Research Express*, **2020**, 7, 095401 | 1.7 | 6 |
| 137 | The Double Wall Boron Nitride Nanotube: Nano-Cylindrical Capacitor. *Oriental Journal of Chemistry*, **2017**, 33, 1213-1222 | 0.8 | 5 |

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| 136 | Quantum Study of Amino Acid Bind to Carbon Nanotube in View of Magnetic Properties. *Fullerenes Nanotubes and Carbon Nanostructures*, **2014**, 22, 709-725 | 1.8 | 5 |
| 135 | Theoretical Studies of Solvent Effects on Binding of Sn (CH3)2(N-acetyl-L-cysteinate) with Single-walled Carbon Nanotube. *Fullerenes Nanotubes and Carbon Nanostructures*, **2013**, 21, 47-63 | 1.8 | 5 |
| 134 | Thermodynamic Study of the Binding of Mercury Ion to Human Growth Hormone at Different Temperatures. *Journal of Solution Chemistry*, **2011**, 40, 575-586 | 1.8 | 5 |
| 133 | Theoretical study of the intermolecular potential energy and second virial coefficient in the mixtures of CH4 and Kr gases: a comparison with experimental data. *Molecular Simulation*, **2010**, 36, 865-870 | 2 | 5 |
| 132 | NMR shielding and a thermodynamic study of the effect of environmental exposure to petrochemical solvent on DPPC, an important component of lung surfactant. *Russian Journal of Physical Chemistry A*, **2007**, 81, 1956-1963 | 0.7 | 5 |
| 131 | Complexation of Tri-o-Propoyl-p-t-Butyl Calix[4]Arene with Alkali Metal Cations in Carbon Tetrachloride Solvent. *Main Group Metal Chemistry*, **2003**, 26, | 1.6 | 5 |
| 130 | Complexes of Adenine and Guanine with Thallium(I). *Main Group Metal Chemistry*, **2004**, 27, | 1.6 | 5 |
| 129 | A Theoretical Study of Metal-Stabilised Rare Tautomers Stability: N4 Metalated Cytosine (M=Be2+, Mg2+, Ca2+, Sr2+ and Ba2+) in Gas Phase and Different Solvents. *Journal of Chemical Research*, **2004**, 2004, 11-18 | 0.6 | 5 |
| 128 | An overview on Coronaviruses family from past to Covid-19: introduce some inhibitors as antiviruses from Gillan□ plants. *Biointerface Research in Applied Chemistry*, **2020**, 10, 5575-5585 | 2.8 | 5 |
| 127 | Kinetic and Mechanism Studies of the Reaction Between L-Tyrosine and Iodine on the Basis of UV-Vis Spectrophotometric Method. *Asian Journal of Biochemistry*, **2008**, 3, 290-296 | 0.1 | 5 |
| 126 | The Effect of Exchange and Correlation on Properties of Carbon Nanotube Structure: A DFT study. *Journal of the Korean Chemical Society*, **2011**, 55, 7-13 | | 5 |
| 125 | Preparation, Characterization and First Application of Graphene Oxide-Metformin-Nickel for the Suzuki Cross-Coupling Reaction. *ChemistrySelect*, **2020**, 5, 211-217 | 1.8 | 5 |
| 124 | Capacitor simulation including of X-doped graphene (X = Li, Be, B) as two electrodes and (h-BN)m (m = 1□4) as the insulator. *Japanese Journal of Applied Physics*, **2015**, 54, 085101 | 1.4 | 4 |
| 123 | Investigation of Langmuir and Freundlich Adsorption Isotherm of Co2+ Ion by Micro Powder of Cedar Leaf. *Oriental Journal of Chemistry*, **2017**, 33, 1569-1574 | 0.8 | 4 |
| 122 | Study of Bio-nano Interaction Outlook of Amino Acids on Single-walled Carbon Nanotubes. *Fullerenes Nanotubes and Carbon Nanostructures*, **2014**, 22, 595-603 | 1.8 | 4 |
| 121 | Harmonic Linear Combination and Normal Mode Analysis of Semiconductor Nanotubes Vibrations. *Journal of Computational and Theoretical Nanoscience*, **2015**, 12, 1030-1039 | 0.3 | 4 |
| 120 | A Dielectric Effect on Normal Mode Analysis and Symmetry of BNNT Nanotube. *Fullerenes Nanotubes and Carbon Nanostructures*, **2011**, 19, 182-196 | 1.8 | 4 |
| 119 | Density Functional Theory Investigation of Natural Bond Orbital Population Analysis and Gauge-Including Atomic Orbital NMR Tensors of K@B36N36. *Journal of Computational and Theoretical Nanoscience*, **2010**, 7, 1147-1158 | 0.3 | 4 |

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| 118 | Density functional B3LYP and B3PW91 studies of the properties of four cyclic organodiboranes with tetramethylene fragments. *Journal of Structural Chemistry*, **2010**, 51, 437-443 | 0.9 | 4 |
| 117 | Thermodynamic Study on the Interaction of Copper Ion with Human Growth Hormone. *Journal of Solution Chemistry*, **2010**, 39, 153-164 | 1.8 | 4 |
| 116 | QM/MM model study on properties and structure of some antibiotics in gas phase: Comparison of energy and NMR chemical shift. *Biochemistry (Moscow)*, **2006**, 71 Suppl 1, S113-22 | 2.9 | 4 |
| 115 | An ab initio quantum chemical investigation of solvent-induced effect on 14N-NQR parameters of alanine, glycine, valine, and serine using a polarizable continuum model. *Russian Journal of Physical Chemistry A*, **2006**, 80, S40-S44 | 0.7 | 4 |
| 114 | Thallium(I) Complexes of Some Sulphur-Containing Ligands. *Main Group Metal Chemistry*, **2003**, 26, 39-48 | 1.6 | 4 |
| 113 | Comparison and Thermodynamic Studies on Complexation of Alanine with Vanadium(V) in Mixed Solvent Systems. *Journal of Chemical & Engineering Data*, **1995**, 40, 419-422 | 2.8 | 4 |
| 112 | Design and Manufacture of Silver-Selective Electrode Based on Single-Walled Carbon Nanotubes. *Oriental Journal of Chemistry*, **2015**, 31, 703-708 | 0.8 | 4 |
| 111 | A Computational Study of Cytotoxicity of Substituted Amides of Pyrazine- 2-carboxylic acids Using QSAR and DFT Based Molecular Surface Electrostatic Potential. *Iranian Journal of Pharmaceutical Research*, **2013**, 12, 745-50 | 1.1 | 4 |
| 110 | Evaluation of Coronavirus Families & Covid-19 Proteins: Molecular Modeling Study. *Biointerface Research in Applied Chemistry*, **2020**, 10, 6039-6057 | 2.8 | 4 |
| 109 | DFT Study on 4(5)-Imidazole-carbaldehyde-N(5)-phenylthiosemicarbazone (ImTPh): NMR Shielding Tensors, Thermodynamic Parameters, NBO Analysis, Molecular Electrostatic Potential (MEP), HOMO and LUMO Studies. *Oriental Journal of Chemistry*, **2014**, 30, 345-350 | 0.8 | 3 |
| 108 | The Electromagnetic Feature of B15N15Hx (x = 0, 4, 8, 12, 16, and 20) Nano Rings: Quantum Theory of Atoms in Molecules/NMR Approach. *Journal of Computational and Theoretical Nanoscience*, **2014**, 11, 1290-1298 | 0.3 | 3 |
| 107 | Nano theoretical studies of fMet-tRNA structure in protein synthesis of prokaryotes and its comparison with the structure of fAla-tRNA. *African Journal of Microbiology Research*, **2011**, 5, 2667-2674 | 0.5 | 3 |
| 106 | Self-Interaction Error of Local Density Functionals for Molecules and Nanotubes. *Fullerenes Nanotubes and Carbon Nanostructures*, **2011**, 19, 692-699 | 1.8 | 3 |
| 105 | A kinetic Monte Carlo simulation study of inositol 1,4,5-trisphosphate receptor (IP3R) calcium release channel. *Computational Biology and Chemistry*, **2007**, 31, 99-109 | 3.6 | 3 |
| 104 | Complexation of alkali metal ions with di and tri-propyl ether of P-tert-butyl-calix[4]arenes: ab initio approach. *Main Group Metal Chemistry*, **2004**, 27, 107-112 | 1.6 | 3 |
| 103 | Molecular dynamic study of human prion protein upon D178N mutation: new perspective to H-bonds, salt bridges and the critical amino acids. *Protein and Peptide Letters*, **2013**, 20, 775-80 | 1.9 | 3 |
| 102 | AIM and NBO analyses on the interaction between SWCNT and cyclophosphamide as an anticancer drug: A density functional theory study. *Journal of Theoretical and Computational Chemistry*, **2015**, 14, 1550021 | 1.8 | 2 |
| 101 | Temperature and Solvent Influence of MWNT (M = 1,2,3) for Nano Drug Delivery and mRNA Binding: A Normal Mode Analysis. *Journal of Computational and Theoretical Nanoscience*, **2015**, 12, 2448-2457 | 0.3 | 2 |

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| 100 | Electronic Structural Investigation of Boron Nitride Nano Cage (B30N20) in Point of Exchange and Correlation Energy. *Journal of Computational and Theoretical Nanoscience*, **2015**, 12, 652-659 | 0.3 | 2 |
| 99 | Neutral Gases Adsorption With Hydrogen on Silicon Nanotubes: A Fuel Cell Invistegation. *Oriental Journal of Chemistry*, **2017**, 33, 1366-1374 | 0.8 | 2 |
| 98 | Adsorption of Thymol Blue and Erythrosine-B on MWCNTs Functionalized by N-(3-nitrobenzylidene)- N'-trimethoxysilylpropyl-ethane-1,2-diamine Equilibrium, Kinetics and Thermodynamic Study. *Oriental Journal of Chemistry*, **2017**, 33, 2542-2550 | 0.8 | 2 |
| 97 | Non Bonded Interactions in cylindrical capacitor of (m, n) @ (m□n□@ (m□n□Three Walled Nano Carbon Nanotubes. *Oriental Journal of Chemistry*, **2017**, 33, 3024-3030 | 0.8 | 2 |
| 96 | Adsorption of Microporous Silica Material (mcm-41) on Graphene Sheet as a Nano-Carrier. *Journal of Computational and Theoretical Nanoscience*, **2016**, 13, 378-387 | 0.3 | 2 |
| 95 | Aromaticity and Induced Current Study of C8H ( n+2)8 (n = □, □, □, 0): In the Viewpoint of Huckel□ Rule. *Journal of Structural Chemistry*, **2019**, 60, 1361-1374 | 0.9 | 2 |
| 94 | The Magnetizability and Chemical Shift Relationship in Carbon Nanotubes with PNP or NPN Junction. *Journal of Computational and Theoretical Nanoscience*, **2014**, 11, 2005-2016 | 0.3 | 2 |
| 93 | Solvent Effect on Aquaporin-4 Channel Membrane: In Point of Nano Biotechnology. *Journal of Computational and Theoretical Nanoscience*, **2015**, 12, 449-458 | 0.3 | 2 |
| 92 | Carbon Nanotubes as the Specific Drug Delivery for Sulfonamides Antibiotics: Instead of Injection. *Journal of Computational and Theoretical Nanoscience*, **2015**, 12, 3808-3816 | 0.3 | 2 |
| 91 | A Nano Capacitor Including Graphene Electrodes and the Hydrogen Insulator. *Journal of Computational and Theoretical Nanoscience*, **2015**, 12, 3473-3481 | 0.3 | 2 |
| 90 | Nano Structure Study on the First Series Transition Cations Inside B16N16-Nanotube in Point of Electromagnetic Interaction. *Fullerenes Nanotubes and Carbon Nanostructures*, **2014**, 22, 798-808 | 1.8 | 2 |
| 89 | Biophysical chemistry of macrocycles for drug delivery: a theoretical study. *Russian Chemical Bulletin*, **2011**, 60, 238-241 | 1.7 | 2 |
| 88 | Electrochemical Oxidation of Catechols in the Presence of Dimethyl Phosphite. *Progress in Reaction Kinetics and Mechanism*, **2012**, 37, 138-146 | 0.5 | 2 |
| 87 | Theoretical study of vitamin properties from combined QM-MM methods: Comparison of chemical shifts and energy. *Russian Journal of Physical Chemistry A*, **2006**, 80, 1061-1068 | 0.7 | 2 |
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