Mehdi Yoosefian

List of Publications by Citations

68 papers	1,749 citations	29 h-index	37 g-index
69 ext. papers	1,999 ext. citations	4.2 avg, IF	5.65 L-index

#	Paper	IF	Citations
68	Optimization of electrocoagulation process for efficient removal of ciprofloxacin antibiotic using iron electrode; kinetic and isotherm studies of adsorption. *Journal of Molecular Liquids*, **2017**, 225, 544-553	6	84
67	ZnO/CNTs nanocomposite/ionic liquid carbon paste electrode for determination of noradrenaline in human samples. *Electrochimica Acta*, **2014**, 123, 456-462	6.7	71
66	A DFT comparative study of single and double SO2 adsorption on Pt-doped and Au-doped single-walled carbon nanotube. *Applied Surface Science*, **2015**, 349, 864-869	6.7	70
65	A voltammetric biosensor based on ionic liquid/NiO nanoparticle modified carbon paste electrode for the determination of nicotinamide adenine dinucleotide (NADH). *Sensors and Actuators B: Chemical*, **2014**, 204, 647-654	8.5	68
64	The hybrid of Pd and SWCNT (Pd loaded on SWCNT) as an efficient sensor for the formaldehyde molecule detection: A DFT study. *Sensors and Actuators B: Chemical*, **2015**, 212, 55-62	8.5	63
63	Powerful greenhouse gas nitrous oxide adsorption onto intrinsic and Pd doped Single walled carbon nanotube. *Applied Surface Science*, **2017**, 392, 225-230	6.7	52
62	The role of solvent polarity in the electronic properties, stability and reactivity trend of a tryptophane/Pd doped SWCNT novel nanobiosensor from polar protic to non-polar solvents. *RSC Advances*, **2016**, 6, 64818-64825	3.7	47
61	Solvent effects on the stability and the electronic properties of histidine/Pd-doped single-walled carbon nanotube biosensor. *Journal of Molecular Liquids*, **2016**, 214, 313-318	6	45
60	Highly Selective Detection of Titanium (III) in Industrial Waste Water Samples Using Meso-octamethylcalix[4]pyrrole-Doped PVC Membrane Ion-Selective Electrode. *Electrochimica Acta* , **2015**, 178, 580-589	6.7	42
59	Nanofilter platform based on functionalized carbon nanotubes for adsorption and elimination of Acrolein, a toxicant in cigarette smoke. *Applied Surface Science*, **2018**, 444, 598-603	6.7	42
58	An Electrochemical Nanosensor for Simultaneous Voltammetric Determination of Ascorbic Acid and Sudan I in Food Samples. *Food Analytical Methods*, **2014**, 7, 2169-2176	3.4	40
57	Density functional theory (DFT) study of a new novel bionanosensor hybrid; tryptophan/Pd doped single walled carbon nanotube. *Physica E: Low-Dimensional Systems and Nanostructures*, **2016**, 81, 116-121	3	39
56	The role of boron nitride nanotube as a new chemical sensor and potential reservoir for hydrogen halides environmental pollutants. *Superlattices and Microstructures*, **2016**, 98, 325-331	2.8	38
55	Ab initio study of Pd-decorated single-walled carbon nanotube with C-vacancy as CO sensor. *Structural Chemistry*, **2014**, 25, 9-19	1.8	38
54	A high efficient nanostructured filter based on functionalized carbon nanotube to reduce the tobacco-specific nitrosamines, NNK. *Applied Surface Science*, **2018**, 434, 134-141	6.7	38
53	Theoretical Description of Substituent Effects in 2,4-Pentanedione: AIM, NBO, and NMR Study. *Bulletin of the Chemical Society of Japan*, **2012**, 85, 87-92	5.1	37
52	Pd-doped single-walled carbon nanotube as a nanobiosensor for histidine amino acid, a DFT study. *RSC Advances*, **2015**, 5, 31172-31178	3.7	35

51	Density functional theory computational study on solvent effect, molecular conformations, energies and intramolecular hydrogen bond strength in different possible nano-conformers of acetaminophen. *Journal of Molecular Liquids*, **2016**, 213, 115-121	6	35
50	The effect of solvents on formaldehyde adsorption performance on pristine and Pd doped on single-walled carbon nanotube using density functional theory. *Journal of Molecular Liquids*, **2017**, 225, 34-41	6	35
49	A molecular study on drug delivery system based on carbon nanotube for the novel norepinephrine prodrug, Droxidopa. *Journal of Molecular Liquids*, **2019**, 284, 258-264	6	33
48	Solvent effects on binding energy, stability order and hydrogen bonding of guanine□ytosine base pair. *Journal of Molecular Liquids*, **2015**, 209, 526-530	6	33
47	Ab initio and DFT computational studies on molecular conformations and strength of the intramolecular hydrogen bond in different conformers of 3-amino-2-iminomethyl acryl aldehyde. *Computational and Theoretical Chemistry*, **2011**, 966, 299-305	2	32
46	A theoretical study on the structure of 2-amino-1,3,4-thiadiazole and its 5-substituted derivatives in the gas phase, water, THF and DMSO solutions. *Journal of Molecular Liquids*, **2015**, 203, 137-142	6	31
45	Hydrogen bond studies in substituted imino-acetaldehyde oxime. *Computational and Theoretical Chemistry*, **2012**, 996, 68-75	2	30
44	Substituent effect on structure, electron density, and intramolecular hydrogen bonding in nitroso-oxime methane. *International Journal of Quantum Chemistry*, **2011**, 111, 3505-3516	2.1	30
43	Boron nitride nanotubes as a nanotransporter for anti-cancer docetaxel drug in water/ethanol solution. *Journal of Molecular Liquids*, **2018**, 271, 151-156	6	30
42	Comprehensive study of the interaction between hydrogen halides and methanol derivatives. *International Journal of Quantum Chemistry*, **2012**, 112, 2782-2786	2.1	29
41	The effects of substitutions on structure, electron density, resonance and intramolecular hydrogen bonding strength in 3-mercapto-propenethial. *Computational and Theoretical Chemistry*, **2010**, 960, 1-9		29
40	Improved electrocoagulation process using chitosan for efficient removal of cefazolin antibiotic from hospital wastewater through sweep flocculation and adsorption: kinetic and isotherm study92, 160-171		29
39	Electronic structures, intramolecular interactions, and aromaticity of substituted 1-(2-iminoethylidene) silan amine: a density functional study. *Structural Chemistry*, **2013**, 24, 123-137	1.8	28
38	Conformational study of the (z)-[(2-iminoethylidone)silyl]amine at the MP2, DFT and G2MP2 levels. *Computational and Theoretical Chemistry*, **2012**, 983, 1-6	2	28
37	The effect of substitution on the intramolecular hydrogen bonding in 3-hydroxy-propenethial. *International Journal of Quantum Chemistry*, **2008**, 108, 1444-1451	2.1	27
36	Ab initio and DFT studies on 1-(thionitrosomethylene) hydrazine: conformers, energies, and intramolecular hydrogen-bond strength. *Structural Chemistry*, **2013**, 24, 1121-1133	1.8	26
35	Encapsulation efficiency of single-walled carbon nanotube for Ifosfamide anti-cancer drug. *Computers in Biology and Medicine*, **2019**, 114, 103433	7	24
34	Nanocarrier for levodopa Parkinson therapeutic drug; comprehensive benserazide analysis. *Artificial Cells, Nanomedicine and Biotechnology*, **2018**, 46, 434-446	6.1	22

33	Comprehensive study of the encapsulation of Lomustine anticancer drug into single walled carbon nanotubes (SWCNTs): Solvent effects, molecular conformations, electronic properties and intramolecular hydrogen bond strength. *Journal of Molecular Liquids*, **2020**, 320, 114285	6	21
32	Leucine/Pd-loaded (5,5) single-walled carbon nanotube matrix as a novel nanobiosensors for in silico detection of protein. *Amino Acids*, **2018**, 50, 653-661	3.5	20
31	Intramolecular hydrogen bonding in derivatives of 3-amino-propenethial. *International Journal of Quantum Chemistry*, **2009**, 109, 1497-1504	2.1	19
30	Ab initio and DFT computational studies on molecular conformations and intramolecular hydrogen bonding in 3-mercapto-but-2-enethial. *Journal of Sulfur Chemistry*, **2010**, 31, 275-285	2.3	18
29	Electronic properties and reactivity trend for defect functionalization of single-walled carbon nanotube with B, Al, Ga atoms. *Synthetic Metals*, **2016**, 221, 242-246	3.6	18
28	Substituent effect on the reaction mechanism of proton transfer in formamide. *International Journal of Quantum Chemistry*, **2012**, 112, 2378-2381	2.1	17
27	Comprehensive experimental and theoretical investigations on chromium (III) trace detection in biological and environmental samples using polymeric membrane sensor. *International Journal of Environmental Analytical Chemistry*, **2019**, 1-16	1.8	17
26	A novel dinuclear schiff base copper complex as an efficient and cost effective catalyst for oxidation of alcohol: Synthesis, crystal structure and theoretical studies. *Journal of Chemical Sciences*, **2015**, 127, 1321-1328	1.8	16
25	Theoretical prediction of chloroform, ethanol, water and DMSO effects on electronic characteristics of Capecitabine different conformers as an anticancer chemotherapy drug. *Journal of Molecular Liquids*, **2018**, 264, 115-118	6	16
24	ANALYSIS OF THE INTRA-MOLECULAR HYDROGEN BOND STRENGTH IN 3-HYDROXY-PROPENETHIAL (HPT). *Journal of Theoretical and Computational Chemistry*, **2009**, 08, 713-732	1.8	16
23	Structural analysis, solvent effects and intramolecular interactions in rilpivirine: A new non-nucleoside reverse transcriptase inhibitor for HIV treatment. *Journal of Molecular Liquids*, **2017**, 246, 124-130	6	15
22	Theoretical study of the effects of substitution, solvation, and structure on the interaction between nitriles and methanol. *International Journal of Quantum Chemistry*, **2012**, 112, 1273-1284	2.1	15
21	THE EFFECT OF SUBSTITUTION ON STRUCTURE, INTRAMOLECULAR HYDROGEN BONDING STRENGTH, ELECTRON DENSITY AND RESONANCE IN 3-AMINO 2-IMINOMETHYL ACRYL ALDEHYDE. *Journal of Theoretical and Computational Chemistry*, **2012**, 11, 925-939	1.8	14
20	Fullerene-C 60 and crown ether doped on C 60 sensors for high sensitive detection of alkali and alkaline earth cations. *Physica E: Low-Dimensional Systems and Nanostructures*, **2017**, 87, 51-58	3	13
19	Conformational study, molecular structure, and SH-N, S-HN intramolecular hydrogen bond in thioformyl-3-aminoacrylaldehyde. *Journal of Sulfur Chemistry*, **2012**, 33, 75-85	2.3	13
18	Theoretical study on aminoacroleine; Density functional theory, atoms in molecules theory and natural bond orbitals studies. *Journal of Chemical Sciences*, **2012**, 124, 731-739	1.8	12
17	Design and development of polymeric micelles as nanocarriers for anti-cancer Ribociclib drug. *Journal of Molecular Liquids*, **2021**, 329, 115574	6	12
16	Ultra-low concentration protein detection based on phenylalanine-Pd/SWCNT as a high sensitivity nanoreceptor.. *RSC Advances*, **2020**, 10, 2650-2660	3.7	10

15	Application of CdO/SWCNTs Nanocomposite Ionic Liquids Carbon Paste Electrode as a Voltammetric Sensor for Determination of Benserazide. *Current Analytical Chemistry*, **2016**, 13, 46-51	1.7	10
14	A theoretical study of solvent effects on the characteristics of the intramolecular hydrogen bond in Droxidopa. *Journal of Chemical Sciences*, **2015**, 127, 1007-1013	1.8	9
13	Carboxylated single-walled carbon nanotubes as a semiconductor for adsorption of acrylamide in mainstream cigarette smoke. *Physica E: Low-Dimensional Systems and Nanostructures*, **2020**, 124, 114299	3	9
12	Solvents effect on the stability and reactivity of Tamoxifen and its nano metabolites as the breast anticancer drug. *Journal of Molecular Liquids*, **2016**, 223, 1151-1157	6	9
11	Simultaneous spectrophotometric determination of the residual of ciprofloxacin, famotidine, and tramadol using magnetic solid phase extraction coupled with multivariate calibration methods. *Microchemical Journal*, **2021**, 160, 105627	4.8	9
10	Doxorubicin delivery to breast cancer cells with transferrin-targeted carbon quantum dots: An in vitro and in silico study. *Journal of Drug Delivery Science and Technology*, **2021**, 62, 102342	4.5	8
9	Molecular dynamics simulations on interaction of ssDNA-causing DM1 with carbon and boron nitride nanotubes to inhibit the formation of CTG repeat secondary structures. *Applied Surface Science*, **2020**, 524, 146572	6.7	7
8	LSPR biosensing for the early-stage prostate cancer detection using hydrogen bonds between PSA and antibody: Molecular dynamic and experimental study. *Journal of Molecular Liquids*, **2021**, 324, 114736	6	7
7	Synthesis and Theoretical Study of Intramolecular Hydrogen Bond at Two Possible Positions in Pyrazolo[1,2-b]phthalazine. *Chinese Journal of Chemistry*, **2012**, 30, 779-784	4.9	5
6	The effect of water/ethanol solvent mixtures on interactions of an antibody selective for wild-type alpha-1-antitrypsin in complex with its antigen. *Journal of Molecular Liquids*, **2020**, 312, 113437	6	4
5	Potential applications of armchair, zigzag, and chiral boron nitride nanotubes as a drug delivery system: Letrozole anticancer drug encapsulation. *Applied Physics A: Materials Science and Processing* , **2021**, 127, 1	2.6	4
4	Water molecules can significantly increase the explosive sensitivity of Nitrotriazolone (NTO) in storage and transport. *Journal of Molecular Liquids*, **2021**, 336, 116372	6	3
3	Molecular Dynamics Simulations of Docetaxel Adsorption on Graphene Quantum Dots Surface Modified by PEG-b-PLA Copolymers.. *Nanomaterials*, **2022**, 12,	5.4	1
2	In silico evaluation of atazanavir as a potential HIV main protease inhibitor and its comparison with new designed analogs.. *Computers in Biology and Medicine*, **2022**, 145, 105523	7	1
1	A comprehensive study of the structure, tautomeric properties, and conformational flexibility of 3-Hydroxy-propeneselenal. *Journal of Chemical Sciences*, **2015**, 127, 999-1006	1.8	