

# Mehdi Yoosefian

## List of Publications by Year in Descending Order

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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.

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	Molecular Dynamics Simulations of Docetaxel Adsorption on Graphene Quantum Dots Surface Modified by PEG-b-PLA Copolymers.. <i>Nanomaterials</i> , <b>2022</b> , 12,	5.4	1
67	In silico evaluation of atazanavir as a potential HIV main protease inhibitor and its comparison with new designed analogs.. <i>Computers in Biology and Medicine</i> , <b>2022</b> , 145, 105523	7	1
66	Potential applications of armchair, zigzag, and chiral boron nitride nanotubes as a drug delivery system: Letrozole anticancer drug encapsulation. <i>Applied Physics A: Materials Science and Processing</i> , <b>2021</b> , 127, 1	2.6	4
65	Doxorubicin delivery to breast cancer cells with transferrin-targeted carbon quantum dots: An in vitro and in silico study. <i>Journal of Drug Delivery Science and Technology</i> , <b>2021</b> , 62, 102342	4.5	8
64	Design and development of polymeric micelles as nanocarriers for anti-cancer Ribociclib drug. <i>Journal of Molecular Liquids</i> , <b>2021</b> , 329, 115574	6	12
63	Simultaneous spectrophotometric determination of the residual of ciprofloxacin, famotidine, and tramadol using magnetic solid phase extraction coupled with multivariate calibration methods. <i>Microchemical Journal</i> , <b>2021</b> , 160, 105627	4.8	9
62	LSPR biosensing for the early-stage prostate cancer detection using hydrogen bonds between PSA and antibody: Molecular dynamic and experimental study. <i>Journal of Molecular Liquids</i> , <b>2021</b> , 324, 114736	6	7
61	Water molecules can significantly increase the explosive sensitivity of Nitrotriazolone (NTO) in storage and transport. <i>Journal of Molecular Liquids</i> , <b>2021</b> , 336, 116372	6	3
60	Carboxylated single-walled carbon nanotubes as a semiconductor for adsorption of acrylamide in mainstream cigarette smoke. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2020</b> , 124, 114299 <sup>3</sup>		9
59	Molecular dynamics simulations on interaction of ssDNA-causing DM1 with carbon and boron nitride nanotubes to inhibit the formation of CTG repeat secondary structures. <i>Applied Surface Science</i> , <b>2020</b> , 524, 146572	6.7	7
58	Ultra-low concentration protein detection based on phenylalanine-Pd/SWCNT as a high sensitivity nanoreceptor.. <i>RSC Advances</i> , <b>2020</b> , 10, 2650-2660	3.7	10
57	The effect of water/ethanol solvent mixtures on interactions of an antibody selective for wild-type alpha-1-antitrypsin in complex with its antigen. <i>Journal of Molecular Liquids</i> , <b>2020</b> , 312, 113437	6	4
56	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. <i>Journal of Molecular Liquids</i> , <b>2020</b> , 320, 114285	6	21
55	Encapsulation efficiency of single-walled carbon nanotube for Ifosfamide anti-cancer drug. <i>Computers in Biology and Medicine</i> , <b>2019</b> , 114, 103433	7	24
54	A molecular study on drug delivery system based on carbon nanotube for the novel norepinephrine prodrug, Droxidopa. <i>Journal of Molecular Liquids</i> , <b>2019</b> , 284, 258-264	6	33
53	Comprehensive experimental and theoretical investigations on chromium (III) trace detection in biological and environmental samples using polymeric membrane sensor. <i>International Journal of Environmental Analytical Chemistry</i> , <b>2019</b> , 1-16	1.8	17
52	Nanocarrier for levodopa Parkinson therapeutic drug; comprehensive benserazide analysis. <i>Artificial Cells, Nanomedicine and Biotechnology</i> , <b>2018</b> , 46, 434-446	6.1	22

51	Theoretical prediction of chloroform, ethanol, water and DMSO effects on electronic characteristics of Capecitabine different conformers as an anticancer chemotherapy drug. <i>Journal of Molecular Liquids</i> , <b>2018</b> , 264, 115-118	6	16
50	Nanofilter platform based on functionalized carbon nanotubes for adsorption and elimination of Acrolein, a toxicant in cigarette smoke. <i>Applied Surface Science</i> , <b>2018</b> , 444, 598-603	6.7	42
49	Leucine/Pd-loaded (5,5) single-walled carbon nanotube matrix as a novel nanobiosensors for in silico detection of protein. <i>Amino Acids</i> , <b>2018</b> , 50, 653-661	3.5	20
48	A high efficient nanostructured filter based on functionalized carbon nanotube to reduce the tobacco-specific nitrosamines, NNK. <i>Applied Surface Science</i> , <b>2018</b> , 434, 134-141	6.7	38
47	Boron nitride nanotubes as a nanotransporter for anti-cancer docetaxel drug in water/ethanol solution. <i>Journal of Molecular Liquids</i> , <b>2018</b> , 271, 151-156	6	30
46	Optimization of electrocoagulation process for efficient removal of ciprofloxacin antibiotic using iron electrode; kinetic and isotherm studies of adsorption. <i>Journal of Molecular Liquids</i> , <b>2017</b> , 225, 544-553	6.3	84
45	Structural analysis, solvent effects and intramolecular interactions in rilpivirine: A new non-nucleoside reverse transcriptase inhibitor for HIV treatment. <i>Journal of Molecular Liquids</i> , <b>2017</b> , 246, 124-130	6	15
44	The effect of solvents on formaldehyde adsorption performance on pristine and Pd doped on single-walled carbon nanotube using density functional theory. <i>Journal of Molecular Liquids</i> , <b>2017</b> , 225, 34-41	6	35
43	Fullerene-C 60 and crown ether doped on C 60 sensors for high sensitive detection of alkali and alkaline earth cations. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2017</b> , 87, 51-58	3	13
42	Powerful greenhouse gas nitrous oxide adsorption onto intrinsic and Pd doped Single walled carbon nanotube. <i>Applied Surface Science</i> , <b>2017</b> , 392, 225-230	6.7	52
41	The role of boron nitride nanotube as a new chemical sensor and potential reservoir for hydrogen halides environmental pollutants. <i>Superlattices and Microstructures</i> , <b>2016</b> , 98, 325-331	2.8	38
40	The role of solvent polarity in the electronic properties, stability and reactivity trend of a tryptophan/Pd doped SWCNT novel nanobiosensor from polar protic to non-polar solvents. <i>RSC Advances</i> , <b>2016</b> , 6, 64818-64825	3.7	47
39	Solvent effects on the stability and the electronic properties of histidine/Pd-doped single-walled carbon nanotube biosensor. <i>Journal of Molecular Liquids</i> , <b>2016</b> , 214, 313-318	6	45
38	Density functional theory computational study on solvent effect, molecular conformations, energies and intramolecular hydrogen bond strength in different possible nano-conformers of acetaminophen. <i>Journal of Molecular Liquids</i> , <b>2016</b> , 213, 115-121	6	35
37	Density functional theory (DFT) study of a new novel bionanosensor hybrid; tryptophan/Pd doped single walled carbon nanotube. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , <b>2016</b> , 81, 116-121	3.1	39
36	Application of CdO/SWCNTs Nanocomposite Ionic Liquids Carbon Paste Electrode as a Voltammetric Sensor for Determination of Benserazide. <i>Current Analytical Chemistry</i> , <b>2016</b> , 13, 46-51	1.7	10
35	Solvents effect on the stability and reactivity of Tamoxifen and its nano metabolites as the breast anticancer drug. <i>Journal of Molecular Liquids</i> , <b>2016</b> , 223, 1151-1157	6	9
34	Electronic properties and reactivity trend for defect functionalization of single-walled carbon nanotube with B, Al, Ga atoms. <i>Synthetic Metals</i> , <b>2016</b> , 221, 242-246	3.6	18

33	Solvent effects on binding energy, stability order and hydrogen bonding of guanine-cytosine base pair. <i>Journal of Molecular Liquids</i> , <b>2015</b> , 209, 526-530	6	33
32	Highly Selective Detection of Titanium (III) in Industrial Waste Water Samples Using Meso-octamethylcalix[4]pyrrole-Doped PVC Membrane Ion-Selective Electrode. <i>Electrochimica Acta</i> , <b>2015</b> , 178, 580-589	6.7	42
31	Pd-doped single-walled carbon nanotube as a nanobiosensor for histidine amino acid, a DFT study. <i>RSC Advances</i> , <b>2015</b> , 5, 31172-31178	3.7	35
30	A novel dinuclear schiff base copper complex as an efficient and cost effective catalyst for oxidation of alcohol: Synthesis, crystal structure and theoretical studies. <i>Journal of Chemical Sciences</i> , <b>2015</b> , 127, 1321-1328	1.8	16
29	A comprehensive study of the structure, tautomeric properties, and conformational flexibility of 3-Hydroxy-propeneselenal. <i>Journal of Chemical Sciences</i> , <b>2015</b> , 127, 999-1006	1.8	
28	A theoretical study of solvent effects on the characteristics of the intramolecular hydrogen bond in Droxidopa. <i>Journal of Chemical Sciences</i> , <b>2015</b> , 127, 1007-1013	1.8	9
27	A DFT comparative study of single and double SO <sub>2</sub> adsorption on Pt-doped and Au-doped single-walled carbon nanotube. <i>Applied Surface Science</i> , <b>2015</b> , 349, 864-869	6.7	70
26	The hybrid of Pd and SWCNT (Pd loaded on SWCNT) as an efficient sensor for the formaldehyde molecule detection: A DFT study. <i>Sensors and Actuators B: Chemical</i> , <b>2015</b> , 212, 55-62	8.5	63
25	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. <i>Journal of Molecular Liquids</i> , <b>2015</b> , 203, 137-142	6	31
24	ZnO/CNTs nanocomposite/ionic liquid carbon paste electrode for determination of noradrenaline in human samples. <i>Electrochimica Acta</i> , <b>2014</b> , 123, 456-462	6.7	71
23	An Electrochemical Nanosensor for Simultaneous Voltammetric Determination of Ascorbic Acid and Sudan I in Food Samples. <i>Food Analytical Methods</i> , <b>2014</b> , 7, 2169-2176	3.4	40
22	A voltammetric biosensor based on ionic liquid/NiO nanoparticle modified carbon paste electrode for the determination of nicotinamide adenine dinucleotide (NADH). <i>Sensors and Actuators B: Chemical</i> , <b>2014</b> , 204, 647-654	8.5	68
21	Ab initio study of Pd-decorated single-walled carbon nanotube with C-vacancy as CO sensor. <i>Structural Chemistry</i> , <b>2014</b> , 25, 9-19	1.8	38
20	Ab initio and DFT studies on 1-(thionitrosomethylene) hydrazine: conformers, energies, and intramolecular hydrogen-bond strength. <i>Structural Chemistry</i> , <b>2013</b> , 24, 1121-1133	1.8	26
19	Electronic structures, intramolecular interactions, and aromaticity of substituted 1-(2-iminoethylidene) silan amine: a density functional study. <i>Structural Chemistry</i> , <b>2013</b> , 24, 123-137	1.8	28
18	Theoretical Description of Substituent Effects in 2,4-Pentanedione: AIM, NBO, and NMR Study. <i>Bulletin of the Chemical Society of Japan</i> , <b>2012</b> , 85, 87-92	5.1	37
17	Conformational study, molecular structure, and S <sub>H</sub> -N, S-H <sub>N</sub> intramolecular hydrogen bond in thioformyl-3-aminoacrylaldehyde. <i>Journal of Sulfur Chemistry</i> , <b>2012</b> , 33, 75-85	2.3	13
16	Conformational study of the (z)-[(2-iminoethylidene)silyl]amine at the MP2, DFT and G2MP2 levels. <i>Computational and Theoretical Chemistry</i> , <b>2012</b> , 983, 1-6	2	28

15	Hydrogen bond studies in substituted imino-acetaldehyde oxime. <i>Computational and Theoretical Chemistry</i> , <b>2012</b> , 996, 68-75	2	30
14	Theoretical study of the effects of substitution, solvation, and structure on the interaction between nitriles and methanol. <i>International Journal of Quantum Chemistry</i> , <b>2012</b> , 112, 1273-1284	2.1	15
13	Substituent effect on the reaction mechanism of proton transfer in formamide. <i>International Journal of Quantum Chemistry</i> , <b>2012</b> , 112, 2378-2381	2.1	17
12	Comprehensive study of the interaction between hydrogen halides and methanol derivatives. <i>International Journal of Quantum Chemistry</i> , <b>2012</b> , 112, 2782-2786	2.1	29
11	Synthesis and Theoretical Study of Intramolecular Hydrogen Bond at Two Possible Positions in Pyrazolo[1,2-b]phthalazine. <i>Chinese Journal of Chemistry</i> , <b>2012</b> , 30, 779-784	4.9	5
10	Theoretical study on ß-aminoacroleine; Density functional theory, atoms in molecules theory and natural bond orbitals studies. <i>Journal of Chemical Sciences</i> , <b>2012</b> , 124, 731-739	1.8	12
9	THE EFFECT OF SUBSTITUTION ON STRUCTURE, INTRAMOLECULAR HYDROGEN BONDING STRENGTH, ELECTRON DENSITY AND RESONANCE IN 3-AMINO 2-IMINOMETHYL ACRYL ALDEHYDE. <i>Journal of Theoretical and Computational Chemistry</i> , <b>2012</b> , 11, 925-939	1.8	14
8	Substituent effect on structure, electron density, and intramolecular hydrogen bonding in nitroso-oxime methane. <i>International Journal of Quantum Chemistry</i> , <b>2011</b> , 111, 3505-3516	2.1	30
7	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. <i>Computational and Theoretical Chemistry</i> , <b>2011</b> , 966, 299-305	2	32
6	Ab initio and DFT computational studies on molecular conformations and intramolecular hydrogen bonding in 3-mercapto-but-2-enethial. <i>Journal of Sulfur Chemistry</i> , <b>2010</b> , 31, 275-285	2.3	18
5	The effects of substitutions on structure, electron density, resonance and intramolecular hydrogen bonding strength in 3-mercapto-propenethial. <i>Computational and Theoretical Chemistry</i> , <b>2010</b> , 960, 1-9		29
4	ANALYSIS OF THE INTRA-MOLECULAR HYDROGEN BOND STRENGTH IN 3-HYDROXY-PROPENETHIAL (HPT). <i>Journal of Theoretical and Computational Chemistry</i> , <b>2009</b> , 08, 713-732 <sup>18</sup>		16
3	Intramolecular hydrogen bonding in derivatives of 3-amino-propenethial. <i>International Journal of Quantum Chemistry</i> , <b>2009</b> , 109, 1497-1504	2.1	19
2	The effect of substitution on the intramolecular hydrogen bonding in 3-hydroxy-propenethial. <i>International Journal of Quantum Chemistry</i> , <b>2008</b> , 108, 1444-1451	2.1	27
1	Improved electrocoagulation process using chitosan for efficient removal of cefazolin antibiotic from hospital wastewater through sweep flocculation and adsorption: kinetic and isotherm study <sup>92</sup> , 160-171		29