Mahmoud Mirzaei

List of Publications by Year
in descending order

111 papers	1,883 citations	201575 27 h-index	345118 36 g-index
111 all docs	111 docs citations	111 times ranked	771 citing authors

#	Article	IF	Citations
1	An efficient BrÃ¸nsted acid ionic liquid catalyzed synthesis of novel spiro1,2,4-triazolidine-5-thiones and their photoluminescence study. Journal of Molecular Structure, 2022, 1249, 131528.	1.8	7
2	Quantum processing of cytidine derivatives and evaluating their in silico interactions with the COVID-19 main protease. Main Group Chemistry, 2022, 21, 263-270.	0.4	8
3	The artificial neural network-based QSPR and DFT prediction of lipophilicity for thioguanine. Main Group Chemistry, 2022, 21, 1091-1103.	0.4	1
4	Interactions of coumarin derivatives with monoamine oxidase biomarkers: In silico approach. Main Group Chemistry, 2022, 21, 641-650.	0.4	3
5	Molecular interactions of indomethacin and amino acids: Computational approach. Main Group Chemistry, 2022, 21, 611-621.	0.4	8
6	Inhibitory effects of curcumin on aldose reductase and cyclooxygenase-2 enzymes. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6424-6430.	2.0	19
7	Formulation and Evaluation of Herbal Hand Sanitizer Based on Stevia (Stevia rebaudiana). Journal of Physics: Conference Series, 2021, 1858, 012053.	0.3	1
8	HOMO-LUMO photosensitization analyses of coronene-cytosine complexes. Main Group Chemistry, 2021, 20, 565-573.	0.4	21
9	DNA Codon Recognition by a Cubane Wire: In Silico Approach. Turkish Computational and Theoretical Chemistry, 2021, 5, 13-19.	0.5	14
10	Structural Analysis of Some Pyrrolopyrimidine Derivatives and Examining their Binding Affinity against Cyclooxygenase-2 Enzyme. Turkish Computational and Theoretical Chemistry, 2021, 5, 14-23.	0.5	3
11	6-Methoxylated Flavonoids: Jacein, and 3-demethyljacein from with Their Endoplasmic Reticulum Stress and Apoptotic Cell Death in Breast Cancer Cells Along with Analysis. Iranian Journal of Pharmaceutical Research, 2021, 20, 417-432.	0.3	0
12	A new sesquiterpenoid from the shoots of Iranian Daphne mucronata Royle with selective inhibition of STAT3 and Smad3/4 cancer-related signaling pathways. DARU, Journal of Pharmaceutical Sciences, 2020, 28, 253-262.	0.9	39
13	Halogenated derivatives of cytidine: Structural analysis and binding affinity. Journal of Theoretical and Computational Chemistry, 2020, 19, 2050033.	1.8	18
14	Lab-in-Silico. Advanced Journal of Chemistry Section B, 2020, 2, 1-2.	0.6	1
15	Non-Covalent Interactions of N-(4-CarboxyPhenyl)Phthalimide with CNTs. Advanced Journal of Chemistry Section B, 2020, 2, 39-45.	0.6	2
16	Computational Studies of Furanone and its 5Methyl/5Phenyl Derivatives. Advanced Journal of Chemistry Section B, 2020, 2, 33.	0.6	0
17	A molecular modelling study of the effects of pivalate ligand substitutions on the magnetic properties of chromium-wheels host complexes. Journal of Molecular Graphics and Modelling, 2019, 87, 41-47.	1.3	1
18	Influence of ligand-bridged substitution on the exchange coupling constant of chromium-wheels host complexes: a density functional theory study. Molecular Physics, 2018, 116, 1306-1319.	0.8	2

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19	Functionalization of (n, 0) CNTs (n = 3â€“16) by uracil: DFT studies. European Physical Journal B, 2018, 91, 1.	0.6	7
20	Surface interaction of H₂O and H₂S onto Ca₁₂O₁₂ nanocluster: Quantumâ€chemical analyses. Surface and Interface Analysis, 2018, 50, 411-419.	0.8	47
21	Electronic structure study of the bimetallic Cu_{1-x}Zn_x alloy thin films. Materials Technology, 2018, 33, 193-197.	1.5	14
22	Chemically uracilâ€“functionalized carbon and silicon carbide nanotubes: Computational studies. Materials Chemistry and Physics, 2018, 205, 164-170.	2.0	12
23	Beryllium oxide (BeO) nanotube provides excellent surface towards adenine adsorption: A dispersion-corrected DFT study in gas and water phases. Current Applied Physics, 2018, 18, 1059-1065.	1.1	56
24	DFT Studies of Single Lithium Adsorption on Coronene. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2018, 73, 685-691.	0.7	14
25	Stevia rebaudiana in Food and Beverage Applications and Its Potential Antioxidant and Antidiabetic: Mini Review. Advanced Science Letters, 2018, 24, 9133-9137.	0.2	6
26	Synthesis and characterization of some novel diaryl urea derivatives bearing quinoxalindione moiety. Research in Pharmaceutical Sciences, 2018, 13, 82.	0.6	8
27	Nickel-decorated B₁₂P₁₂ nanoclusters as a strong adsorbent for SO₂ adsorption: Quantum chemical calculations. Canadian Journal of Physics, 2017, 95, 958-962.	0.4	44
28	DFT studies of stabilities and properties for X3Y6Z9 borazineâ€“like structures (X= B/Al, Y= N/P, Z= H/Me). Superlattices and Microstructures, 2017, 109, 360-365.	1.4	4
29	Application of pristine and Ni-decorated B 12 P 12 nano-clusters as superior media for acetylene and ethylene adsorption: DFT calculations. Computational and Theoretical Chemistry, 2017, 1109, 1-9.	1.1	69
30	DFT Studies of Graphene-Functionalised Derivatives of Capecitabine. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2017, 72, 1131-1138.	0.7	11
31	Protection capacity of mosquito repellent ink from citronella (Cymbopogon nardus L.) and clove leaf oils (Syzygium aromaticum) againts Aedes aegypti. AIP Conference Proceedings, 2017, , .	0.3	3
32	Non-Covalent Functionalisation of C₃₀ Fullerene by Pyrrole-n-Carboxylic Acid (n=2, 3): Density Functional Theory Studies. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2017, 73, 51-56.	0.7	12
33	Docking study, synthesis and antimicrobial evaluation of some novel 4-anilinoquinazoline derivatives. Research in Pharmaceutical Sciences, 2017, 12, 425.	0.6	24
34	Synthesis, characterization, cytotoxic screening, and density functional theory studies of new derivatives of quinazolin-4(3H)-one Schiff bases. Research in Pharmaceutical Sciences, 2017, 12, 444.	0.6	7
35	Biological evaluation, docking and molecular dynamic simulation of some novel diaryl urea derivatives bearing quinoxalindione moiety. Research in Pharmaceutical Sciences, 2017, 12, 500.	0.6	9
36	Relaxations of fluorouracil tautomers by decorations of fullerene-like SiCs: DFT studies. Physics Letters, Section A: General, Atomic and Solid State Physics, 2016, 380, 2160-2166.	0.9	42

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37	DFT explorations of quadrupole coupling constants for planar 5-fluorouracil pairs. Computational and Theoretical Chemistry, 2016, 1090, 67-73.	1.1	35
38	Synthesis, vibrational, electrostatic potential and NMR studies of (E and Z) 1-(4-chloro-3-nitrophenyl)-3-(2-methoxyphenyl)triazene: Combined experimental and DFT approaches. Journal of Molecular Structure, 2016, 1125, 247-259.	1.8	6
39	Explorations of Crystalline Effects on 4-(Benzyloxy)Benzaldehyde Properties. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2015, 70, 1013-1018.	0.7	4
40	DFT studies of CNTâ€“functionalized uracil-acetate hybrids. Physica E: Low-Dimensional Systems and Nanostructures, 2015, 73, 105-109.	1.3	8
41	Covalent addition of chitosan to graphene sheets: Density functional theory explorations of quadrupole coupling constants. Superlattices and Microstructures, 2015, 88, 56-61.	1.4	13
42	DFT studies of 5-fluorouracil tautomers on a silicon graphene nanosheet. Superlattices and Microstructures, 2015, 85, 784-788.	1.4	38
43	Formations of CNT modified 5-(halogen)uracil hybrids: DFT studies. Superlattices and Microstructures, 2014, 65, 375-379.	1.4	7
44	Formations of boron-doped and nitrogen-doped silicon nanotubes: DFT studies. Superlattices and Microstructures, 2013, 64, 52-57.	1.4	10
45	Uracil-functionalized ultra-small (n,0) boron nitride nanotubes (n=3â€“6): Computational studies. Superlattices and Microstructures, 2013, 57, 44-50.	1.4	12
46	Formation of a peptide assisted bi-graphene and its properties: DFT studies. Superlattices and Microstructures, 2013, 54, 47-53.	1.4	7
47	Investigating pristine and carbon-decorated silicon nanocones: DFT studies. Superlattices and Microstructures, 2013, 58, 130-134.	1.4	5
48	Modified (n, 0) BN nanotubes (n=3â€“10) by acetic acids: DFT studies. Superlattices and Microstructures, 2013, 55, 1-7.	1.4	17
49	A cytosine-assisted carbon nanotubes junction: DFT studies. Superlattices and Microstructures, 2012, 52, 158-164.	1.4	5
50	Modifying a graphene layer by a thymine or a uracil nucleobase: DFT studies. Superlattices and Microstructures, 2012, 52, 306-311.	1.4	22
51	Silicon carbide nanocones: Computational analysis of chemical shieldings for pristine and boron/nitrogen decorated models. Superlattices and Microstructures, 2012, 52, 523-527.	1.4	7
52	Covalent hybridizations of carbon nanotubes through peptide linkages: A density functional approach. Computational and Theoretical Chemistry, 2012, 981, 47-51.	1.1	7
53	Computational studies of the purine-functionalized graphene sheets. Superlattices and Microstructures, 2012, 52, 612-617.	1.4	37
54	Boron nitride nanotubes with quadrangular cross sections: Density functional studies. Superlattices and Microstructures, 2012, 52, 648-652.	1.4	2

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55	Covalent attachments of boron nitride nanotubes through a carboxylic linker: Density functional studies. Solid State Sciences, 2012, 14, 689-692.	1.5	10
56	Studying (n, 0) and (m,m) GaP nanotubes (nÂ=Â3â€“10 and mÂ=Â2â€“6) through DFT calculations of Ga-69 quadrupole coupling constants. Solid State Sciences, 2012, 14, 801-804.	1.5	12
57	Density functional studies of oxygen-terminations versus hydrogen-terminations in carbon and silicon nanotubes. Solid State Sciences, 2012, 14, 874-879.	1.5	8
58	Chemical shielding properties for BN, BP, AlN, and AlP nanocones: DFT studies. Superlattices and Microstructures, 2012, 51, 809-813.	1.4	9
59	A computational study of aluminum phosphide nanotubes. International Journal of Quantum Chemistry, 2011, 111, 3851-3855.	1.0	3
60	Density functional studies of the fluorine-terminated boron nitride nanotubes through computations of quadrupole coupling constants. Computational and Theoretical Chemistry, 2011, 977, 29-33.	1.1	9
61	Computational NMR studies of silicon nanotubes. Computational and Theoretical Chemistry, 2011, 978, 123-125.	1.1	12
62	The C-doped AlP nanotubes: A computational study. Solid State Sciences, 2011, 13, 244-250.	1.5	34
63	Investigating electronic and structural properties of nitrogen-doped silicon carbide nanotubes through density functional calculations of chemical shielding parameters. Solid State Sciences, 2011, 13, 1251-1255.	1.5	8
64	Computational studies of effects of tubular lengths on the NMR properties of pristine and carbon decorated boron phosphide nanotubes. Solid State Sciences, 2011, 13, 1926-1930.	1.5	16
65	Carbon doped boron phosphide nanotubes: A computational study. Journal of Molecular Modeling, 2011, 17, 89-96.	0.8	32
66	A computational study of atomic oxygen-doped silicon carbide nanotubes. Journal of Molecular Modeling, 2011, 17, 527-531.	0.8	8
67	Covalent hybridization of CNT by thymine and uracil: A computational study. Journal of Molecular Modeling, 2011, 17, 695-699.	0.8	38
68	DFT calculations of NMR properties for GaP nanotubes. Monatshefte FÃ¼r Chemie, 2011, 142, 111-114.	0.9	13
69	A DFT study of N-doped AlP nanotubes. Monatshefte FÃ¼r Chemie, 2011, 142, 115-118.	0.9	9
70	A theoretical study of boron-doped aluminum phosphide nanotubes. Computational and Theoretical Chemistry, 2011, 963, 294-297.	1.1	6
71	A computational study of silicon-doped aluminum phosphide nanotubes. Physica B: Condensed Matter, 2011, 406, 84-87.	1.3	3
72	A computational study of gallium phosphide nanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2011, 43, 1343-1345.	1.3	15

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73	COMPUTATIONAL STUDY OF A CNT-URACIL-CNT COMPOUND. Modern Physics Letters B, 2011, 25, 1335-1341.	1.0	5
74	A Computational NMR Study of Boron Phosphide Nanotubes. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2010, 65, 844-848.	0.7	14
75	The Al-doped BN nanotubes: A DFT study. Computational and Theoretical Chemistry, 2010, 942, 83-87.	1.5	41
76	Aluminum phosphide nanotubes: Density functional calculations of aluminum-27 and phosphorus-31 chemical shielding parameters. Computational and Theoretical Chemistry, 2010, 951, 69-71.	1.5	36
77	Computational NQR study of a boron nitride nanocone. Monatshefte FÃ¼r Chemie, 2010, 141, 305-307.	0.9	3
78	A computational study of oxygen-termination of a (6,0) boron nitride nanotube. Monatshefte FÃ¼r Chemie, 2010, 141, 491-494.	0.9	12
79	SiC-doped boron nitride nanotubes: computations of 11B and 14N quadrupole coupling constants. Monatshefte FÃ¼r Chemie, 2010, 141, 611-614.	0.9	6
80	SiC nanotubes: DFT calculations of 29Si and 13C NMR properties. Monatshefte FÃ¼r Chemie, 2010, 141, 941-943.	0.9	6
81	Electronic structure of sulfur terminated zigzag boron nitride nanotube: A computational study. Solid State Sciences, 2010, 12, 1337-1340.	1.5	7
82	Computational studies on boron nitride and boron phosphide nanotubes: Density functional calculations of boron-11 electric field gradient tensors. Physica E: Low-Dimensional Systems and Nanostructures, 2010, 42, 1667-1669.	1.3	40
83	The NMR parameters of the SiC-doped BN nanotubes: A DFT study. Physica E: Low-Dimensional Systems and Nanostructures, 2010, 42, 1954-1957.	1.3	19
84	Sulfur doping at the tips of (6,0) boron nitride nanotube: A DFT study. Physica E: Low-Dimensional Systems and Nanostructures, 2010, 42, 2147-2150.	1.3	28
85	Computational investigation of the electronic and structural properties of ultra small-diameter boron nitride nanotubes. Physica B: Condensed Matter, 2010, 405, 2542-2544.	1.3	12
86	Computations of the quadrupole coupling constants in aluminum doped boron nitride nanotubes. Physica B: Condensed Matter, 2010, 405, 3991-3994.	1.3	5
87	The B-doped SiC nanotubes: A computational study. Computational and Theoretical Chemistry, 2010, 953, 134-138.	1.5	26
88	An electronic structure study of O-terminated zigzag BN nanotubes: Density functional calculations of the quadrupole coupling constants. Solid State Communications, 2010, 150, 1238-1240.	0.9	12
89	Defective BN Nanotubes: A Density Functional Theory Study of B-11 and N-14 NQR Parameters. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2009, 64, 251-256.	0.7	8
90	Density Functional Study of Defects in Boron Nitride Nanotubes. Zeitschrift Fur Physikalische Chemie, 2009, 223, 815-823.	1.4	26

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91	Calculation of chemical shielding in C-doped zigzag BN nanotubes. Monatshefte FÃ¼r Chemie, 2009, 140, 1275-1278.	0.9	34
92	DFT calculations of B-11 and N-15 NMR parameters in BN nanocone. Computational and Theoretical Chemistry, 2009, 913, 207-209.	1.5	15
93	The carbon-doped (4,4) boron nitride nanotube: A computational NMR approach. Physica E: Low-Dimensional Systems and Nanostructures, 2009, 41, 883-885.	1.3	44
94	Determination of Pseudoephedrine Hydrochloride in Some Pharmaceutical Drugs by Potentiometric Membrane Sensor Based on Pseudoephedrineâ€“Phosphotungstate Ion Pair. Analytical Letters, 2009, 42, 870-880.	1.0	17
95	Study of hydrogen bonds in N-methylacetamide by DFT calculations of oxygen, nitrogen, and hydrogen solid-state NMR parameters. Structural Chemistry, 2008, 19, 225-232.	1.0	10
96	A computational NQR study on the hydrogenâ€bonded lattice of cytosineâ€5â€acetic acid. Journal of Computational Chemistry, 2008, 29, 832-838.	1.5	32
97	Density functional calculations of 14N and 11B NQR parameters in the H-capped (6,0) and (4,4) single-walled BN nanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2008, 40, 800-804.	1.3	38
98	Density functional study of zigzag BN nanotubes with equivalent ends. Physica E: Low-Dimensional Systems and Nanostructures, 2008, 40, 3060-3063.	1.3	37
99	A computational NMR study on zigzag aluminum nitride nanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2008, 41, 209-212.	1.3	33
100	The C-doped zigzag AlN nanotube: A computational NMR study. Chemical Physics Letters, 2008, 461, 246-248.	1.2	45
101	Hydrogen bond interactions in sulfamerazine: DFT study of the O-17, N-14, and H-2 electric field gradient tensors. Chemical Physics, 2008, 351, 159-162.	0.9	10
102	CARBON-SUBSTITUTING IN (4,4) BORON NITRIDE NANOTUBE: DENSITY FUNCTIONAL STUDY OF BORON-11 AND NITROGEN-14 ELECTRIC FIELD GRADIENT TENSORS. Journal of Theoretical and Computational Chemistry, 2008, 07, 447-455.	1.8	4
103	Density Functional Study of the Influence of Carbon Doping on the Aluminum-27 and Nitrogen-14 Electric Field Gradient Tensors in (10, 0) Single-Walled Aluminum Nitride Nanotube. Zeitschrift Fur Physikalische Chemie, 2008, 222, 1569-1577.	1.4	0
104	AlN Nanotubes: A DFT Study of Al-27 and N-14 Electric Field Gradient Tensors. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2007, 62, 711-715.	0.7	16
105	Influence of C-Doping on the B-11 and N-14 Quadrupole Coupling Constants in Boron-Nitride Nanotubes: A DFT Study. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2007, 62, 56-60.	0.7	31
106	Study of hydrogen bonds in 1-methyluracil by DFT calculations of oxygen, nitrogen, and hydrogen quadrupole coupling constants and isotropic chemical shifts. Chemical Physics Letters, 2007, 438, 304-307.	1.2	24
107	A density functional study of 17O, 14N and 2H electric field gradient tensors in the real crystalline structure of Î±-glycine. Biophysical Chemistry, 2007, 125, 179-183.	1.5	32
108	Investigation of Câ€“Hâ€¦OC and Nâ€“Hâ€¦OC hydrogen-bonding interactions in crystalline thymine by DFT calculations of O-17, N-14 and H-2 NQR parameters. Biophysical Chemistry, 2007, 125, 411-415.	1.5	31

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109	A Systematic Investigation of Hydrogen-Bonding Effects on the17O,14N, and2H Nuclear Quadrupole Resonance Parameters of Anhydrous and Monohydrated Cytosine Crystalline Structures:Â A Density Functional Theory Study. Journal of Physical Chemistry B, 2006, 110, 10991-10996.	1.2	27
110	An Investigation of Hydrogen-Bonding Effects on the Nitrogen and Hydrogen Electric Field Gradient and Chemical Shielding Tensors in the 9-Methyladenine Real Crystalline Structure:Â A Density Functional Theory Study. Journal of Physical Chemistry A, 2006, 110, 4833-4838.	1.1	61
111	The Câ€“HÂ·Â·Â·O Hydrogen Bonding Effects on the ¹⁷O Electric Field Gradient and Chemical Shielding Tensors in Crystalline 1-Methyluracil: A DFT Study. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2006, 61, 383-388.	0.7	12