Mahmoud Mirzaei

List of Publications by Year
in descending order

111 papers	1,883 citations	201674 27 h-index	345221 36 g-index
111 all docs	111 docs citations	111 times ranked	771 citing authors

#	Article	IF	Citations
1	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.	2.5	69
2	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.	2.5	61
3	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.	2.4	56
4	Surface interaction of H₂O and H₂S onto Ca₁₂O₁₂ nanocluster: Quantumâ€chemical analyses. Surface and Interface Analysis, 2018, 50, 411-419.	1.8	47
5	The C-doped zigzag AlN nanotube: A computational NMR study. Chemical Physics Letters, 2008, 461, 246-248.	2.6	45
6	The carbon-doped (4,4) boron nitride nanotube: A computational NMR approach. Physica E: Low-Dimensional Systems and Nanostructures, 2009, 41, 883-885.	2.7	44
7	Nickel-decorated B₁₂P₁₂ nanoclusters as a strong adsorbent for SO₂ adsorption: Quantum chemical calculations. Canadian Journal of Physics, 2017, 95, 958-962.	1.1	44
8	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.	2.1	42
9	The Al-doped BN nanotubes: A DFT study. Computational and Theoretical Chemistry, 2010, 942, 83-87.	1.5	41
10	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.	2.7	40
11	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.	2.0	39
12	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.	2.7	38
13	Covalent hybridization of CNT by thymine and uracil: A computational study. Journal of Molecular Modeling, 2011, 17, 695-699.	1.8	38
14	DFT studies of 5-fluorouracil tautomers on a silicon graphene nanosheet. Superlattices and Microstructures, 2015, 85, 784-788.	3.1	38
15	Density functional study of zigzag BN nanotubes with equivalent ends. Physica E: Low-Dimensional Systems and Nanostructures, 2008, 40, 3060-3063.	2.7	37
16	Computational studies of the purine-functionalized graphene sheets. Superlattices and Microstructures, 2012, 52, 612-617.	3.1	37
17	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
18	DFT explorations of quadrupole coupling constants for planar 5-fluorouracil pairs. Computational and Theoretical Chemistry, 2016, 1090, 67-73.	2.5	35

#	Article	IF	Citations
19	Calculation of chemical shielding in C-doped zigzag BN nanotubes. Monatshefte FÃ¼r Chemie, 2009, 140, 1275-1278.	1.8	34
20	The C-doped AlP nanotubes: A computational study. Solid State Sciences, 2011, 13, 244-250.	3.2	34
21	A computational NMR study on zigzag aluminum nitride nanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2008, 41, 209-212.	2.7	33
22	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.	2.8	32
23	A computational NQR study on the hydrogenâ€bonded lattice of cytosineâ€5â€acetic acid. Journal of Computational Chemistry, 2008, 29, 832-838.	3.3	32
24	Carbon doped boron phosphide nanotubes: A computational study. Journal of Molecular Modeling, 2011, 17, 89-96.	1.8	32
25	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.	1.5	31
26	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.	2.8	31
27	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.	2.7	28
28	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.	2.6	27
29	Density Functional Study of Defects in Boron Nitride Nanotubes. Zeitschrift Fur Physikalische Chemie, 2009, 223, 815-823.	2.8	26
30	The B-doped SiC nanotubes: A computational study. Computational and Theoretical Chemistry, 2010, 953, 134-138.	1.5	26
31	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.	2.6	24
32	Docking study, synthesis and antimicrobial evaluation of some novel 4-anilinoquinazoline derivatives. Research in Pharmaceutical Sciences, 2017, 12, 425.	1.8	24
33	Modifying a graphene layer by a thymine or a uracil nucleobase: DFT studies. Superlattices and Microstructures, 2012, 52, 306-311.	3.1	22
34	HOMO-LUMO photosensitization analyses of coronene-cytosine complexes. Main Group Chemistry, 2021, 20, 565-573.	0.8	21
35	The NMR parameters of the SiC-doped BN nanotubes: A DFT study. Physica E: Low-Dimensional Systems and Nanostructures, 2010, 42, 1954-1957.	2.7	19
36	Inhibitory effects of curcumin on aldose reductase and cyclooxygenase-2 enzymes. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6424-6430.	3.5	19

#	Article	IF	Citations
37	Halogenated derivatives of cytidine: Structural analysis and binding affinity. Journal of Theoretical and Computational Chemistry, 2020, 19, 2050033.	1.8	18
38	Determination of Pseudoephedrine Hydrochloride in Some Pharmaceutical Drugs by Potentiometric Membrane Sensor Based on Pseudoephedrineâ€“Phosphotungstate Ion Pair. Analytical Letters, 2009, 42, 870-880.	1.8	17
39	Modified (n, 0) BN nanotubes (n=3â€“10) by acetic acids: DFT studies. Superlattices and Microstructures, 2013, 55, 1-7.	3.1	17
40	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.	1.5	16
41	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.	3.2	16
42	DFT calculations of B-11 and N-15 NMR parameters in BN nanocone. Computational and Theoretical Chemistry, 2009, 913, 207-209.	1.5	15
43	A computational study of gallium phosphide nanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2011, 43, 1343-1345.	2.7	15
44	A Computational NMR Study of Boron Phosphide Nanotubes. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2010, 65, 844-848.	1.5	14
45	Electronic structure study of the bimetallic Cu_{1-x}Zn_x alloy thin films. Materials Technology, 2018, 33, 193-197.	3.0	14
46	DFT Studies of Single Lithium Adsorption on Coronene. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2018, 73, 685-691.	1.5	14
47	DNA Codon Recognition by a Cubane Wire: In Silico Approach. Turkish Computational and Theoretical Chemistry, 2021, 5, 13-19.	0.5	14
48	DFT calculations of NMR properties for GaP nanotubes. Monatshefte FÃ¼r Chemie, 2011, 142, 111-114.	1.8	13
49	Covalent addition of chitosan to graphene sheets: Density functional theory explorations of quadrupole coupling constants. Superlattices and Microstructures, 2015, 88, 56-61.	3.1	13
50	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.	1.5	12
51	A computational study of oxygen-termination of a (6,0) boron nitride nanotube. Monatshefte FÃ¼r Chemie, 2010, 141, 491-494.	1.8	12
52	Computational investigation of the electronic and structural properties of ultra small-diameter boron nitride nanotubes. Physica B: Condensed Matter, 2010, 405, 2542-2544.	2.7	12
53	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.	1.9	12
54	Computational NMR studies of silicon nanotubes. Computational and Theoretical Chemistry, 2011, 978, 123-125.	2.5	12

#	Article	IF	Citations
55	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.	3.2	12
56	Uracil-functionalized ultra-small (n,0) boron nitride nanotubes (n=3â€“6): Computational studies. Superlattices and Microstructures, 2013, 57, 44-50.	3.1	12
57	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.	1.5	12
58	Chemically uracilâ€“functionalized carbon and silicon carbide nanotubes: Computational studies. Materials Chemistry and Physics, 2018, 205, 164-170.	4.0	12
59	DFT Studies of Graphene-Functionalised Derivatives of Capecitabine. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2017, 72, 1131-1138.	1.5	11
60	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.	2.0	10
61	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.	1.9	10
62	Covalent attachments of boron nitride nanotubes through a carboxylic linker: Density functional studies. Solid State Sciences, 2012, 14, 689-692.	3.2	10
63	Formations of boron-doped and nitrogen-doped silicon nanotubes: DFT studies. Superlattices and Microstructures, 2013, 64, 52-57.	3.1	10
64	Density functional studies of the fluorine-terminated boron nitride nanotubes through computations of quadrupole coupling constants. Computational and Theoretical Chemistry, 2011, 977, 29-33.	2.5	9
65	A DFT study of N-doped AlP nanotubes. Monatshefte FÃ¼r Chemie, 2011, 142, 115-118.	1.8	9
66	Chemical shielding properties for BN, BP, AlN, and AlP nanocones: DFT studies. Superlattices and Microstructures, 2012, 51, 809-813.	3.1	9
67	Biological evaluation, docking and molecular dynamic simulation of some novel diaryl urea derivatives bearing quinoxalindione moiety. Research in Pharmaceutical Sciences, 2017, 12, 500.	1.8	9
68	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.	1.5	8
69	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.	3.2	8
70	A computational study of atomic oxygen-doped silicon carbide nanotubes. Journal of Molecular Modeling, 2011, 17, 527-531.	1.8	8
71	Density functional studies of oxygen-terminations versus hydrogen-terminations in carbon and silicon nanotubes. Solid State Sciences, 2012, 14, 874-879.	3.2	8
72	DFT studies of CNTâ€“functionalized uracil-acetate hybrids. Physica E: Low-Dimensional Systems and Nanostructures, 2015, 73, 105-109.	2.7	8

#	Article	IF	Citations
73	Synthesis and characterization of some novel diaryl urea derivatives bearing quinoxalindione moiety. Research in Pharmaceutical Sciences, 2018, 13, 82.	1.8	8
74	Quantum processing of cytidine derivatives and evaluating their in silico interactions with the COVID-19 main protease. Main Group Chemistry, 2022, 21, 263-270.	0.8	8
75	Molecular interactions of indomethacin and amino acids: Computational approach. Main Group Chemistry, 2022, 21, 611-621.	0.8	8
76	Electronic structure of sulfur terminated zigzag boron nitride nanotube: A computational study. Solid State Sciences, 2010, 12, 1337-1340.	3.2	7
77	Silicon carbide nanocones: Computational analysis of chemical shieldings for pristine and boron/nitrogen decorated models. Superlattices and Microstructures, 2012, 52, 523-527.	3.1	7
78	Covalent hybridizations of carbon nanotubes through peptide linkages: A density functional approach. Computational and Theoretical Chemistry, 2012, 981, 47-51.	2.5	7
79	Formation of a peptide assisted bi-graphene and its properties: DFT studies. Superlattices and Microstructures, 2013, 54, 47-53.	3.1	7
80	Formations of CNT modified 5-(halogen)uracil hybrids: DFT studies. Superlattices and Microstructures, 2014, 65, 375-379.	3.1	7
81	Functionalization of (n, 0) CNTs (n = 3â€“16) by uracil: DFT studies. European Physical Journal B, 2018, 91, 1.	1.5	7
82	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.	3.6	7
83	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.	1.8	7
84	SiC-doped boron nitride nanotubes: computations of 11B and 14N quadrupole coupling constants. Monatshefte FÃ¼r Chemie, 2010, 141, 611-614.	1.8	6
85	SiC nanotubes: DFT calculations of 29Si and 13C NMR properties. Monatshefte FÃ¼r Chemie, 2010, 141, 941-943.	1.8	6
86	A theoretical study of boron-doped aluminum phosphide nanotubes. Computational and Theoretical Chemistry, 2011, 963, 294-297.	2.5	6
87	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.	3.6	6
88	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
89	Computations of the quadrupole coupling constants in aluminum doped boron nitride nanotubes. Physica B: Condensed Matter, 2010, 405, 3991-3994.	2.7	5
90	COMPUTATIONAL STUDY OF A CNT-URACIL-CNT COMPOUND. Modern Physics Letters B, 2011, 25, 1335-1341.	1.9	5

#	Article	IF	Citations
91	A cytosine-assisted carbon nanotubes junction: DFT studies. Superlattices and Microstructures, 2012, 52, 158-164.	3.1	5
92	Investigating pristine and carbon-decorated silicon nanocones: DFT studies. Superlattices and Microstructures, 2013, 58, 130-134.	3.1	5
93	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
94	Explorations of Crystalline Effects on 4-(Benzyloxy)Benzaldehyde Properties. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2015, 70, 1013-1018.	1.5	4
95	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.	3.1	4
96	Computational NQR study of a boron nitride nanocone. Monatshefte FÃ¼r Chemie, 2010, 141, 305-307.	1.8	3
97	A computational study of aluminum phosphide nanotubes. International Journal of Quantum Chemistry, 2011, 111, 3851-3855.	2.0	3
98	A computational study of silicon-doped aluminum phosphide nanotubes. Physica B: Condensed Matter, 2011, 406, 84-87.	2.7	3
99	Protection capacity of mosquito repellent ink from citronella (Cymbopogon nardus L.) and clove leaf oils (Syzygium aromaticum) againts Aedes aegypti. AIP Conference Proceedings, 2017, , .	0.4	3
100	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
101	Interactions of coumarin derivatives with monoamine oxidase biomarkers: In silico approach. Main Group Chemistry, 2022, 21, 641-650.	0.8	3
102	Boron nitride nanotubes with quadrangular cross sections: Density functional studies. Superlattices and Microstructures, 2012, 52, 648-652.	3.1	2
103	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.	1.7	2
104	Non-Covalent Interactions of N-(4-CarboxyPhenyl)Phthalimide with CNTs. Advanced Journal of Chemistry Section B, 2020, 2, 39-45.	0.6	2
105	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.	2.4	1
106	Formulation and Evaluation of Herbal Hand Sanitizer Based on Stevia (Stevia rebaudiana). Journal of Physics: Conference Series, 2021, 1858, 012053.	0.4	1
107	Lab-in-Silico. Advanced Journal of Chemistry Section B, 2020, 2, 1-2.	0.6	1
108	The artificial neural network-based QSPR and DFT prediction of lipophilicity for thioguanine. Main Group Chemistry, 2022, 21, 1091-1103.	0.8	1

#	Article	IF	Citations
109	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.	2.8	0
110	Computational Studies of Furanone and its 5Methyl/5Phenyl Derivatives. Advanced Journal of Chemistry Section B, 2020, 2, 33.	0.6	0
111	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.	0.5	0