

Mahmoud Mirzaei

List of Publications by Year in descending order

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#	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. <i>Computational and Theoretical Chemistry</i> , 2017, 1109, 1-9.	1.1	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: A Density Functional Theory Study. <i>Journal of Physical Chemistry A</i> , 2006, 110, 4833-4838.	1.1	61
3	Beryllium oxide (BeO) nanotube provides excellent surface towards adenine adsorption: A dispersion-corrected DFT study in gas and water phases. <i>Current Applied Physics</i> , 2018, 18, 1059-1065.	1.1	56
4	Surface interaction of H ₂ O and H ₂ S onto Ca ₁₂ O ₁₂ nanocluster: Quantum chemical analyses. <i>Surface and Interface Analysis</i> , 2018, 50, 411-419.	0.8	47
5	The C-doped zigzag AlN nanotube: A computational NMR study. <i>Chemical Physics Letters</i> , 2008, 461, 246-248.	1.2	45
6	The carbon-doped (4,4) boron nitride nanotube: A computational NMR approach. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2009, 41, 883-885.	1.3	44
7	Nickel-decorated B ₁₂ P ₁₂ nanoclusters as a strong adsorbent for SO ₂ adsorption: Quantum chemical calculations. <i>Canadian Journal of Physics</i> , 2017, 95, 958-962.	0.4	44
8	Relaxations of fluorouracil tautomers by decorations of fullerene-like SiCs: DFT studies. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2016, 380, 2160-2166.	0.9	42
9	The Al-doped BN nanotubes: A DFT study. <i>Computational and Theoretical Chemistry</i> , 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. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2010, 42, 1667-1669.	1.3	40
11	A new sesquiterpenoid from the shoots of Iranian <i>Daphne mucronata</i> Royle with selective inhibition of STAT3 and Smad3/4 cancer-related signaling pathways. <i>DARU, Journal of Pharmaceutical Sciences</i> , 2020, 28, 253-262.	0.9	39
12	Density functional calculations of ¹⁴ N and ¹¹ B NQR parameters in the H-capped (6,0) and (4,4) single-walled BN nanotubes. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2008, 40, 800-804.	1.3	38
13	Covalent hybridization of CNT by thymine and uracil: A computational study. <i>Journal of Molecular Modeling</i> , 2011, 17, 695-699.	0.8	38
14	DFT studies of 5-fluorouracil tautomers on a silicon graphene nanosheet. <i>Superlattices and Microstructures</i> , 2015, 85, 784-788.	1.4	38
15	Density functional study of zigzag BN nanotubes with equivalent ends. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2008, 40, 3060-3063.	1.3	37
16	Computational studies of the purine-functionalized graphene sheets. <i>Superlattices and Microstructures</i> , 2012, 52, 612-617.	1.4	37
17	Aluminum phosphide nanotubes: Density functional calculations of aluminum-27 and phosphorus-31 chemical shielding parameters. <i>Computational and Theoretical Chemistry</i> , 2010, 951, 69-71.	1.5	36
18	DFT explorations of quadrupole coupling constants for planar 5-fluorouracil pairs. <i>Computational and Theoretical Chemistry</i> , 2016, 1090, 67-73.	1.1	35

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19	Calculation of chemical shielding in C-doped zigzag BN nanotubes. Monatshefte für Chemie, 2009, 140, 1275-1278.	0.9	34
20	The C-doped AlP nanotubes: A computational study. Solid State Sciences, 2011, 13, 244-250.	1.5	34
21	A computational NMR study on zigzag aluminum nitride nanotubes. Physica E: Low-Dimensional Systems and Nanostructures, 2008, 41, 209-212.	1.3	33
22	A density functional study of ^{17}O , ^{14}N and ^2H electric field gradient tensors in the real crystalline structure of L-glycine. Biophysical Chemistry, 2007, 125, 179-183.	1.5	32
23	A computational NQR study on the hydrogen-bonded lattice of cytosine-acetic acid. Journal of Computational Chemistry, 2008, 29, 832-838.	1.5	32
24	Carbon doped boron phosphide nanotubes: A computational study. Journal of Molecular Modeling, 2011, 17, 89-96.	0.8	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.	0.7	31
26	Investigation of C-H \cdots O and N-H \cdots O 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
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.	1.3	28
28	A Systematic Investigation of Hydrogen-Bonding Effects on the ^{17}O , ^{14}N , and ^2H Nuclear Quadrupole Resonance Parameters of Anhydrous and Monohydrated Cytosine Crystalline Structures: A Density Functional Theory Study. Journal of Physical Chemistry B, 2006, 110, 10991-10996.	1.2	27
29	Density Functional Study of Defects in Boron Nitride Nanotubes. Zeitschrift Fur Physikalische Chemie, 2009, 223, 815-823.	1.4	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.	1.2	24
32	Docking study, synthesis and antimicrobial evaluation of some novel 4-anilinoquinazoline derivatives. Research in Pharmaceutical Sciences, 2017, 12, 425.	0.6	24
33	Modifying a graphene layer by a thymine or a uracil nucleobase: DFT studies. Superlattices and Microstructures, 2012, 52, 306-311.	1.4	22
34	HOMO-LUMO photosensitization analyses of coronene-cytosine complexes. Main Group Chemistry, 2021, 20, 565-573.	0.4	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.	1.3	19
36	Inhibitory effects of curcumin on aldose reductase and cyclooxygenase-2 enzymes. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6424-6430.	2.0	19

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37	Halogenated derivatives of cytidine: Structural analysis and binding affinity. <i>Journal of Theoretical and Computational Chemistry</i> , 2020, 19, 2050033.	1.8	18
38	Determination of Pseudoephedrine Hydrochloride in Some Pharmaceutical Drugs by Potentiometric Membrane Sensor Based on Pseudoephedrine α -Phosphotungstate Ion Pair. <i>Analytical Letters</i> , 2009, 42, 870-880.	1.0	17
39	Modified (n, 0) BN nanotubes (n=3 \leq 10) by acetic acids: DFT studies. <i>Superlattices and Microstructures</i> , 2013, 55, 1-7.	1.4	17
40	AlN Nanotubes: A DFT Study of Al-27 and N-14 Electric Field Gradient Tensors. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2007, 62, 711-715.	0.7	16
41	Computational studies of effects of tubular lengths on the NMR properties of pristine and carbon decorated boron phosphide nanotubes. <i>Solid State Sciences</i> , 2011, 13, 1926-1930.	1.5	16
42	DFT calculations of B-11 and N-15 NMR parameters in BN nanocone. <i>Computational and Theoretical Chemistry</i> , 2009, 913, 207-209.	1.5	15
43	A computational study of gallium phosphide nanotubes. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2011, 43, 1343-1345.	1.3	15
44	A Computational NMR Study of Boron Phosphide Nanotubes. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2010, 65, 844-848.	0.7	14
45	Electronic structure study of the bimetallic Cu _{1-x} Zn _x alloy thin films. <i>Materials Technology</i> , 2018, 33, 193-197.	1.5	14
46	DFT Studies of Single Lithium Adsorption on Coronene. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2018, 73, 685-691.	0.7	14
47	DNA Codon Recognition by a Cubane Wire: In Silico Approach. <i>Turkish Computational and Theoretical Chemistry</i> , 2021, 5, 13-19.	0.5	14
48	DFT calculations of NMR properties for GaP nanotubes. <i>Monatshefte Für Chemie</i> , 2011, 142, 111-114.	0.9	13
49	Covalent addition of chitosan to graphene sheets: Density functional theory explorations of quadrupole coupling constants. <i>Superlattices and Microstructures</i> , 2015, 88, 56-61.	1.4	13
50	The C-H \cdots O Hydrogen Bonding Effects on the ¹⁷ O Electric Field Gradient and Chemical Shielding Tensors in Crystalline 1-Methyluracil: A DFT Study. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2006, 61, 383-388.	0.7	12
51	A computational study of oxygen-termination of a (6,0) boron nitride nanotube. <i>Monatshefte Für Chemie</i> , 2010, 141, 491-494.	0.9	12
52	Computational investigation of the electronic and structural properties of ultra small-diameter boron nitride nanotubes. <i>Physica B: Condensed Matter</i> , 2010, 405, 2542-2544.	1.3	12
53	An electronic structure study of O-terminated zigzag BN nanotubes: Density functional calculations of the quadrupole coupling constants. <i>Solid State Communications</i> , 2010, 150, 1238-1240.	0.9	12
54	Computational NMR studies of silicon nanotubes. <i>Computational and Theoretical Chemistry</i> , 2011, 978, 123-125.	1.1	12

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55	Studying (n, 0) and (m,m) GaP nanotubes ($n=3$ and $m=2$) through DFT calculations of Ga-69 quadrupole coupling constants. <i>Solid State Sciences</i> , 2012, 14, 801-804.	1.5	12
56	Uracil-functionalized ultra-small (n,0) boron nitride nanotubes ($n=3$): Computational studies. <i>Superlattices and Microstructures</i> , 2013, 57, 44-50.	1.4	12
57	Non-Covalent Functionalisation of C_{30} Fullerene by Pyrrole-Carboxylic Acid ($n=2, 3$): Density Functional Theory Studies. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2017, 73, 51-56.	0.7	12
58	Chemically uracil-functionalized carbon and silicon carbide nanotubes: Computational studies. <i>Materials Chemistry and Physics</i> , 2018, 205, 164-170.	2.0	12
59	DFT Studies of Graphene-Functionalised Derivatives of Capecitabine. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2017, 72, 1131-1138.	0.7	11
60	Study of hydrogen bonds in N-methylacetamide by DFT calculations of oxygen, nitrogen, and hydrogen solid-state NMR parameters. <i>Structural Chemistry</i> , 2008, 19, 225-232.	1.0	10
61	Hydrogen bond interactions in sulfamerazine: DFT study of the O-17, N-14, and H-2 electric field gradient tensors. <i>Chemical Physics</i> , 2008, 351, 159-162.	0.9	10
62	Covalent attachments of boron nitride nanotubes through a carboxylic linker: Density functional studies. <i>Solid State Sciences</i> , 2012, 14, 689-692.	1.5	10
63	Formations of boron-doped and nitrogen-doped silicon nanotubes: DFT studies. <i>Superlattices and Microstructures</i> , 2013, 64, 52-57.	1.4	10
64	Density functional studies of the fluorine-terminated boron nitride nanotubes through computations of quadrupole coupling constants. <i>Computational and Theoretical Chemistry</i> , 2011, 977, 29-33.	1.1	9
65	A DFT study of N-doped AlP nanotubes. <i>Monatshefte Für Chemie</i> , 2011, 142, 115-118.	0.9	9
66	Chemical shielding properties for BN, BP, AlN, and AlP nanocones: DFT studies. <i>Superlattices and Microstructures</i> , 2012, 51, 809-813.	1.4	9
67	Biological evaluation, docking and molecular dynamic simulation of some novel diaryl urea derivatives bearing quinoxalindione moiety. <i>Research in Pharmaceutical Sciences</i> , 2017, 12, 500.	0.6	9
68	Defective BN Nanotubes: A Density Functional Theory Study of B-11 and N-14 NQR Parameters. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2009, 64, 251-256.	0.7	8
69	Investigating electronic and structural properties of nitrogen-doped silicon carbide nanotubes through density functional calculations of chemical shielding parameters. <i>Solid State Sciences</i> , 2011, 13, 1251-1255.	1.5	8
70	A computational study of atomic oxygen-doped silicon carbide nanotubes. <i>Journal of Molecular Modeling</i> , 2011, 17, 527-531.	0.8	8
71	Density functional studies of oxygen-terminations versus hydrogen-terminations in carbon and silicon nanotubes. <i>Solid State Sciences</i> , 2012, 14, 874-879.	1.5	8
72	DFT studies of CNT-functionalized uracil-acetate hybrids. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2015, 73, 105-109.	1.3	8

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73	Synthesis and characterization of some novel diaryl urea derivatives bearing quinoxalindione moiety. <i>Research in Pharmaceutical Sciences</i> , 2018, 13, 82.	0.6	8
74	Quantum processing of cytidine derivatives and evaluating their in silico interactions with the COVID-19 main protease. <i>Main Group Chemistry</i> , 2022, 21, 263-270.	0.4	8
75	Molecular interactions of indomethacin and amino acids: Computational approach. <i>Main Group Chemistry</i> , 2022, 21, 611-621.	0.4	8
76	Electronic structure of sulfur terminated zigzag boron nitride nanotube: A computational study. <i>Solid State Sciences</i> , 2010, 12, 1337-1340.	1.5	7
77	Silicon carbide nanocones: Computational analysis of chemical shieldings for pristine and boron/nitrogen decorated models. <i>Superlattices and Microstructures</i> , 2012, 52, 523-527.	1.4	7
78	Covalent hybridizations of carbon nanotubes through peptide linkages: A density functional approach. <i>Computational and Theoretical Chemistry</i> , 2012, 981, 47-51.	1.1	7
79	Formation of a peptide assisted bi-graphene and its properties: DFT studies. <i>Superlattices and Microstructures</i> , 2013, 54, 47-53.	1.4	7
80	Formations of CNT modified 5-(halogen)uracil hybrids: DFT studies. <i>Superlattices and Microstructures</i> , 2014, 65, 375-379.	1.4	7
81	Functionalization of (n, 0) CNTs (n = 3-16) by uracil: DFT studies. <i>European Physical Journal B</i> , 2018, 91, 1.	0.6	7
82	An efficient Brønsted acid ionic liquid catalyzed synthesis of novel spiro1,2,4-triazolidine-5-thiones and their photoluminescence study. <i>Journal of Molecular Structure</i> , 2022, 1249, 131528.	1.8	7
83	Synthesis, characterization, cytotoxic screening, and density functional theory studies of new derivatives of quinoxalin-4(3H)-one Schiff bases. <i>Research in Pharmaceutical Sciences</i> , 2017, 12, 444.	0.6	7
84	SiC-doped boron nitride nanotubes: computations of 11B and 14N quadrupole coupling constants. <i>Monatshefte für Chemie</i> , 2010, 141, 611-614.	0.9	6
85	SiC nanotubes: DFT calculations of 29Si and 13C NMR properties. <i>Monatshefte für Chemie</i> , 2010, 141, 941-943.	0.9	6
86	A theoretical study of boron-doped aluminum phosphide nanotubes. <i>Computational and Theoretical Chemistry</i> , 2011, 963, 294-297.	1.1	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. <i>Journal of Molecular Structure</i> , 2016, 1125, 247-259.	1.8	6
88	<i>Stevia rebaudiana</i> in Food and Beverage Applications and Its Potential Antioxidant and Antidiabetic: Mini Review. <i>Advanced Science Letters</i> , 2018, 24, 9133-9137.	0.2	6
89	Computations of the quadrupole coupling constants in aluminum doped boron nitride nanotubes. <i>Physica B: Condensed Matter</i> , 2010, 405, 3991-3994.	1.3	5
90	COMPUTATIONAL STUDY OF A CNT-URACIL-CNT COMPOUND. <i>Modern Physics Letters B</i> , 2011, 25, 1335-1341.	1.0	5

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91	A cytosine-assisted carbon nanotubes junction: DFT studies. Superlattices and Microstructures, 2012, 52, 158-164.	1.4	5
92	Investigating pristine and carbon-decorated silicon nanocones: DFT studies. Superlattices and Microstructures, 2013, 58, 130-134.	1.4	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.	0.7	4
95	DFT studies of stabilities and properties for X ₃ Y ₆ Z ₉ borazine-like structures (X= B/Al, Y= N/P, Z= H/Me). Superlattices and Microstructures, 2017, 109, 360-365.	1.4	4
96	Computational NQR study of a boron nitride nanocone. Monatshefte für Chemie, 2010, 141, 305-307.	0.9	3
97	A computational study of aluminum phosphide nanotubes. International Journal of Quantum Chemistry, 2011, 111, 3851-3855.	1.0	3
98	A computational study of silicon-doped aluminum phosphide nanotubes. Physica B: Condensed Matter, 2011, 406, 84-87.	1.3	3
99	Protection capacity of mosquito repellent ink from citronella (<i>Cymbopogon nardus</i> L.) and clove leaf oils (<i>Syzygium aromaticum</i>) against <i>Aedes aegypti</i> . AIP Conference Proceedings, 2017, , .	0.3	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.	0.4	3
102	Boron nitride nanotubes with quadrangular cross sections: Density functional studies. Superlattices and Microstructures, 2012, 52, 648-652.	1.4	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.	0.8	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.	1.3	1
106	Formulation and Evaluation of Herbal Hand Sanitizer Based on Stevia (<i>Stevia rebaudiana</i>). Journal of Physics: Conference Series, 2021, 1858, 012053.	0.3	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.	0.4	1

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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.	1.4	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.	0.3	0