

Mohammad Taghi Baei

List of Publications by Citations

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120
papers

2,108
citations

26
h-index

40
g-index

122
ext. papers

2,338
ext. citations

2.3
avg, IF

5.38
L-index

#	Paper	IF	Citations
120	Theoretical study of CO adsorption on the surface of BN, AlN, BP and ALP nanotubes. <i>Surface Science</i> , 2012 , 606, 981-985	1.8	125
119	AlN nanotube as a potential electronic sensor for nitrogen dioxide. <i>Microelectronics Journal</i> , 2012 , 43, 452-455	1.8	84
118	Carbon nitride nanotube as a sensor for alkali and alkaline earth cations. <i>Applied Surface Science</i> , 2013 , 264, 699-706	6.7	80
117	B-doping makes the carbon nanocones sensitive towards NO molecules. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 2012 , 377, 107-111	2.3	79
116	Electronic sensor for sulfide dioxide based on AlN nanotubes: a computational study. <i>Journal of Molecular Modeling</i> , 2012 , 18, 4745-50	2	70
115	A computational study of AlN nanotube as an oxygen detector. <i>Chinese Chemical Letters</i> , 2012 , 23, 965-968	2.8	66
114	Sensitivity of BN nano-cages to caffeine and nicotine molecules. <i>Superlattices and Microstructures</i> , 2014 , 76, 315-325	2.8	65
113	Phenol adsorption study on pristine, Ga-, and In-doped (4,4) armchair single-walled boron nitride nanotubes. <i>Computational and Theoretical Chemistry</i> , 2012 , 997, 63-69	2	60
112	Carbon nanocone as an ammonia sensor: DFT studies. <i>Structural Chemistry</i> , 2013 , 24, 1099-1103	1.8	58
111	A computational study of adenine, uracil, and cytosine adsorption upon AlN and BN nano-cages. <i>Physica B: Condensed Matter</i> , 2014 , 444, 6-13	2.8	54
110	ZnO Nanocluster as a Potential Catalyst for Dissociation of H ₂ S Molecule. <i>Journal of Cluster Science</i> , 2013 , 24, 341-347	3	54
109	Adsorption of cyanogen chloride over Al- and Ga-doped BN nanotubes. <i>Superlattices and Microstructures</i> , 2014 , 75, 564-575	2.8	52
108	A DFT study of 5-fluorouracil adsorption on the pure and doped BN nanotubes. <i>Journal of Physics and Chemistry of Solids</i> , 2015 , 86, 57-64	3.9	48
107	Adsorption properties of N ₂ O on (6,0), (7,0), and (8,0) zigzag single-walled boron nitride nanotubes: A computational study. <i>Computational and Theoretical Chemistry</i> , 2011 , 970, 30-35	2	46
106	Adsorption of chemical warfare agents over C ₂₄ fullerene: Effects of decoration of cobalt. <i>Journal of Alloys and Compounds</i> , 2018 , 735, 2148-2161	5.7	41
105	Phenol interaction with different nano-cages with and without an electric field: a DFT study. <i>Structural Chemistry</i> , 2015 , 26, 685-693	1.8	38
104	B ₁₂ N ₁₂ sodalite like cage as potential sensor for hydrogen cyanide. <i>Computational and Theoretical Chemistry</i> , 2013 , 1024, 28-33	2	35

103	Formation and electronic structure of C ₂₀ fullerene transition metal clusters. <i>Monatshefte für Chemie</i> , 2014 , 145, 1401-1405	1.4	33
102	The electronic and structural properties of BN and BP nano-cages interacting with OCN radical DFT study. <i>Journal of Physics and Chemistry of Solids</i> , 2014 , 75, 1099-1105	3.9	33
101	Al ₁₂ N ₁₂ nanocage as a potential sensor for phosgene detection. <i>Canadian Journal of Chemistry</i> , 2014 , 92, 605-610	0.9	29
100	Transition metal atom adsorptions on a boron nitride nanocage. <i>Structural Chemistry</i> , 2013 , 24, 1039-1044	4.8	28
99	Adsorption of CO molecule on AlN nanotubes by parallel electric field. <i>Journal of Molecular Modeling</i> , 2013 , 19, 859-70	2	27
98	Theoretical Study of Thiazole Adsorption on the (6,0) zigzag Single-Walled Boron Nitride Nanotube. <i>Bulletin of the Korean Chemical Society</i> , 2012 , 33, 3285-3292	1.2	27
97	The study of SCN ⁻ adsorption on B ₁₂ N ₁₂ and B ₁₆ N ₁₆ nano-cages. <i>Superlattices and Microstructures</i> , 2014 , 75, 716-724	2.8	26
96	Nitrous oxide adsorption on pristine and Si-doped AlN nanotubes. <i>Journal of Molecular Modeling</i> , 2013 , 19, 943-9	2	26
95	A density functional theory study on acetylene-functionalized BN nanotubes. <i>Structural Chemistry</i> , 2013 , 24, 1007-1013	1.8	26
94	Adsorption phenomena of gas molecules upon Ga-doped BN nanotubes: A DFT study. <i>Applied Surface Science</i> , 2014 , 295, 18-25	6.7	25
93	A DFT Study on CO ₂ Interaction with a BN Nano-Cage. <i>Bulletin of the Korean Chemical Society</i> , 2012 , 33, 3338-3342	1.2	25
92	First-Principles Study of NO ₂ Adsorption on C ₂₀ Fullerene. <i>Heteroatom Chemistry</i> , 2013 , 24, 516-523	1.2	23
91	First Principles Study on Encapsulation of Alkali Metals into ZnO Nanocage. <i>Chinese Journal of Chemical Physics</i> , 2012 , 25, 671-675	0.9	21
90	Selective adsorption behavior of BC ₂ N nanotubes toward fluoride and chloride. <i>Solid State Communications</i> , 2013 , 159, 8-12	1.6	20
89	Adsorption properties of OCN radical on (6,0), (8,0), and (10,0) zigzag single-walled carbon nanotubes: a density functional study. <i>Monatshefte für Chemie</i> , 2011 , 142, 1-4	1.4	20
88	Quantum chemical analysis on hydrogenated Zn ₁₂ O ₁₂ nanoclusters. <i>Comptes Rendus Chimie</i> , 2013 , 16, 122-128	2.7	19
87	Fluorination of the exterior surface of AlN nanotube: A DFT study. <i>Superlattices and Microstructures</i> , 2013 , 53, 9-15	2.8	19
86	The influence of NH ₃ -attaching on the NMR and NQR parameters in the (6,0) zigzag single-walled BPNTs: a density functional study. <i>Computational and Theoretical Chemistry</i> , 2011 , 967, 179-184	2	19

85	Co-adsorption of CO molecules at the open ends of MgO nanotubes. <i>Structural Chemistry</i> , 2012 , 23, 1981-1986	1.8	18
84	BN Nanotube Serving as a Gas Chemical Sensor for N ₂ O by Parallel Electric Field. <i>Journal of Cluster Science</i> , 2016 , 27, 1081-1096	3	18
83	Zn ₁₂ O ₁₂ Fullerene-like Cage as a Potential Sensor for SO ₂ Detection. <i>Adsorption Science and Technology</i> , 2013 , 31, 469-476	3.6	17
82	Zn ₁₂ O ₁₂ nano-cage as a promising adsorbent for CS ₂ capture. <i>Superlattices and Microstructures</i> , 2013 , 58, 198-204	2.8	17
81	Theoretical Study of Phenol Adsorption on Pristine, Ga-Doped, and Pd-Decorated (6,0) Zigzag Single-Walled Boron Phosphide Nanotubes. <i>Journal of Cluster Science</i> , 2013 , 24, 49-60	3	16
80	Effect of Gallium Doping on Electronic and Structural Properties (6,0) Zigzag Silicon Carbide Nanotube as a p-Semiconductor. <i>Journal of Cluster Science</i> , 2012 , 23, 1119-1132	3	16
79	Remove of toxic pyridine from environmental systems by using B ₁₂ N ₁₂ nano-cage. <i>Superlattices and Microstructures</i> , 2013 , 58, 31-37	2.8	16
78	Sb(V) removal from copper electrorefining electrolyte: Comparative study by different sorbents. <i>Transactions of Nonferrous Metals Society of China</i> , 2017 , 27, 440-449	3.3	15
77	Theoretical study on pure and doped B ₁₂ N ₁₂ fullerenes as thiophene sensor. <i>Adsorption</i> , 2018 , 24, 585-593	3	15
76	NMR and NQR parameters of the SiC-doped on the (4,4) armchair single-walled BPNT: a computational study. <i>Journal of Molecular Modeling</i> , 2012 , 18, 881-9	2	15
75	Adsorption of nitrous oxide on the (6,0) magnesium oxide nanotube. <i>Chinese Chemical Letters</i> , 2012 , 23, 1275-1278	8.1	15
74	The Al-Doped Carbon Nanotubes: A DFT Study. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2012 , 20, 681-687	1.8	15
73	DFT Study of CO ₂ Adsorption on the Zn ₁₂ O ₁₂ Nano-cage. <i>Bulletin of the Korean Chemical Society</i> , 2013 , 34, 3722-3726	1.2	15
72	First Principles Calculations of Electric Field Effect on the (6,0) Zigzag Single-Walled Silicon Carbide Nanotube for use in Nano-Electronic Circuits. <i>Journal of Cluster Science</i> , 2013 , 24, 591-604	3	14
71	Theoretical study of cyano radical adsorption on (6,0) zigzag single-walled carbon nanotube. <i>Monatshefte für Chemie</i> , 2012 , 143, 1463-1470	1.4	14
70	The Ge-doped (6,0) zigzag single-walled boron phosphide nanotubes: A computational study. <i>Computational and Theoretical Chemistry</i> , 2011 , 972, 14-19	2	14
69	Adsorption properties of N ₂ O on (6,0), (7,0), (8,0), and Al-doped (6,0) zigzag single-walled carbon nanotubes: a density functional study. <i>Monatshefte für Chemie</i> , 2011 , 142, 573-578	1.4	14
68	Silicon-doping makes the B ₁₂ N ₁₂ insulator to an n or p-semiconductor. <i>Superlattices and Microstructures</i> , 2013 , 60, 437-442	2.8	13

67	Interaction of pure and metal atom substituted carbon nanocages with CNCl: a DFT study. <i>Russian Journal of Physical Chemistry B</i> , 2017 , 11, 354-360	1.2	12
66	First-principles calculations of structural stability, electronic, and electrical responses of GeC nanotube under electric field effect for use in nanoelectronic devices. <i>Superlattices and Microstructures</i> , 2012 , 52, 1119-1130	2.8	12
65	Electronic, Energetic, and Geometric Properties of Methylene-Functionalized C60. <i>Journal of Cluster Science</i> , 2013 , 24, 669-678	3	12
64	NMR and NQR parameters of Si-doped (6,0) zigzag single-walled boron phosphide nanotubes: a density functional study. <i>Monatshefte für Chemie</i> , 2011 , 142, 1097-1104	1.4	12
63	Adsorption properties of hydrazine on pristine and Si-doped Al12N12 nano-cage. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2016 , 191, 702-708	1	11
62	Electric field effect on the zigzag (6,0) single-wall BC2N nanotube for use in nano-electronic circuits. <i>Journal of Molecular Modeling</i> , 2013 , 19, 97-107	2	11
61	Al12N12 nanocage as potential adsorbent for removal of acetone from environmental systems. <i>Monatshefte für Chemie</i> , 2015 , 146, 891-896	1.4	10
60	Adsorption mechanism of single OCN and SCN upon single-walled BP nanotubes. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2014 , 59, 66-74	3	10
59	Electric field effect on (6,0) zigzag single-walled aluminum nitride nanotube. <i>Journal of Molecular Modeling</i> , 2012 , 18, 4477-89	2	10
58	NMR parameters of SiC-doped (6,0) zigzag single-walled boron phosphide nanotubes: a density functional study. <i>Monatshefte für Chemie</i> , 2011 , 142, 783-788	1.4	10
57	Structure, stability, and electronic properties of ALP nanocages evolved from the world's smallest caged fullerene C20: A computational study at DFT. <i>Journal of Molecular Structure</i> , 2018 , 1159, 118-134	3-4	9
56	A DFT Study on Structure and Electronic Properties of BN Nanostructures Adsorbed with Dopamine. <i>Computation</i> , 2019 , 7, 61	2.2	9
55	Characterization of C20 fullerene and its isolated C20- n Gen derivatives (n=1-5) by alternating germanium atom(s) in equatorial position: A DFT survey. <i>Heteroatom Chemistry</i> , 2018 , 29, e21410	1.2	8
54	Computational study of OCN chemisorption over AlN nanostructures. <i>Superlattices and Microstructures</i> , 2014 , 72, 370-382	2.8	8
53	Adsorption properties of H2O2 trapped inside a boron phosphide nanotube. <i>Monatshefte für Chemie</i> , 2012 , 143, 37-41	1.4	8
52	Covalent Functionalization of Zn12O12 Nanocluster with Thiophene. <i>Journal of Cluster Science</i> , 2013 , 24, 749-756	3	8
51	Adsorption and electronic structure study of thiazole on the (6,0) zigzag single-walled boron phosphide nanotube. <i>Journal of Sulfur Chemistry</i> , 2013 , 34, 407-420	2.3	8
50	Covalent functionalization of AlN nanotubes with acetylene. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2013 , 47, 147-151	3	8

49	Adsorption and Electronic Structure Study of Imidazole on (6,0) Zigzag Single-Walled Boron Nitride Nanotube. <i>Journal of Cluster Science</i> , 2012 , 24, 31	3	8
48	Computational studies on aluminum nitride and aluminum phosphide nanotubes: density functional calculations of 27Al electric field gradient tensors. <i>Monatshefte Für Chemie</i> , 2012 , 143, 545-549	1.4	8
47	Adsorption properties of SCN ⁻ on (6,0), (7,0), (8,0), and Al-doped (6,0) zigzag single-walled carbon nanotubes: a density functional study. <i>Monatshefte Für Chemie</i> , 2011 , 142, 979-984	1.4	8
46	DFT study of the adsorption of H ₂ O ₂ inside and outside Al ₁₂ N ₁₂ nano-cage. <i>Russian Journal of Physical Chemistry A</i> , 2017 , 91, 1527-1534	0.7	7
45	Influence of the adsorption of toxic agents on the optical and electronic properties of B ₁₂ N ₁₂ fullerene in the presence and absence of an external electric field. <i>New Journal of Chemistry</i> , 2020 , 44, 14513-14528	3.6	7
44	Molecular Modeling and Simulation of glycine functionalized B ₁₂ N ₁₂ and B ₁₆ N ₁₆ nanoclusters as potential inhibitors of proinflammatory cytokines. <i>Journal of Molecular Liquids</i> , 2021 , 343, 117494	6	7
43	Sensitivity of C ₂₄ Fullerene to Nicotine Molecule. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2015 , 23, 874-877	1.8	6
42	Si-Doped B ₁₂ N ₁₂ Nanocage as an Adsorbent for Dissociation of N ₂ O to N ₂ Molecule. <i>Heteroatom Chemistry</i> , 2013 , 24, 476-481	1.2	6
41	Electronic structure study of Si-doped (4,4) armchair single-walled boron phosphide nanotube as a semiconductor. <i>Monatshefte Für Chemie</i> , 2012 , 143, 1627-1635	1.4	6
40	Effects of Zinc Binding on the Structure and Stability of Glycylglycine Dipeptide: A Computational Study. <i>E-Journal of Chemistry</i> , 2012 , 9, 1244-1250		6
39	Ge-doped (4,4) armchair single-walled boron phosphide nanotube as a semiconductor: a computational study. <i>Monatshefte Für Chemie</i> , 2012 , 143, 881-889	1.4	6
38	Adsorption Properties of Oxygen on H-Capped (5, 5) Boron Nitride Nanotube (BNNT)- A Density Functional Theory. <i>E-Journal of Chemistry</i> , 2011 , 8, 609-614		6
37	Structural and electronic properties of XY-doped (AlN, AlP, GaN, GaP) C ₅₈ fullerenes: a DFT study. <i>Russian Journal of Inorganic Chemistry</i> , 2017 , 62, 1067-1076	1.5	5
36	Covalent Functionalization of Pristine and Ga-Doped Boron Phosphide Nanotubes with Imidazole. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2014 , 189, 453-464	1	5
35	Adsorption properties and quantum molecular descriptors of OCN ⁻ adsorbed on (6,0), (7,0), and (8,0) zigzag single-walled boron nitride nanotubes: a computational study. <i>Monatshefte Für Chemie</i> , 2012 , 143, 989-995	1.4	5
34	Adsorption of Thiophene on Aluminum Nitride Nanotubes. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2013 , 188, 1172-1177	1	5
33	A density-functional theory of hydrogen adsorption on indium nitride nanotubes. <i>Russian Journal of Inorganic Chemistry</i> , 2017 , 62, 325-335	1.5	4
32	C ₃₀ B ₁₅ N ₁₅ Heterofullerene as a Potential Electronic Sensor for NO Detection. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2015 , 23, 153-157	1.8	4

31	Improvement of Antioxidative Activity of Apigenin by B12N12 Nanocluster: Antioxidative Mechanism Analysis. <i>ChemistrySelect</i> , 2020 , 5, 1829-1836	1.8	4
30	Electronic Structure Study of Gallium and Indium Doped (4,4) armchair Single-Walled Boron Nitride Nanotubes for Production of Solid-State Devices. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2015 , 23, 68-77	1.8	4
29	Quantum molecular descriptors and adsorption properties of SCN on (6,0), (7,0), (8,0), and Ga-doped (6,0) zigzag single-walled boron nitride nanotubes: a computational study. <i>Monatshefte für Chemie</i> , 2012 , 143, 1115-1121	1.4	4
28	A Dielectric Effect on Normal Mode Analysis and Symmetry of BNNT Nanotube. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2011 , 19, 182-196	1.8	4
27	DFT Study of the Interactions of Carbon Monoxide with Pd-Decorated (6,0) Single-Walled Carbon Nanotube. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2013 , 21, 12-18	1.8	3
26	Ionic liquid as an effective green media for the synthesis of (5Z, 8Z)-7H-pyrido[2,3-d]azepine derivatives and recyclable Fe ₃ O ₄ /TiO ₂ /multi-wall carbon nanotubes magnetic nanocomposites as high performance organometallic nanocatalyst. <i>Molecular Diversity</i> , 2021 , 1	3.1	3
25	Adsorption of the urea molecule on the B ₁₂ N ₁₂ nanocage. <i>Turkish Journal of Chemistry</i> , 2014 , 38, 531-537	1	2
24	Ab Initio and DFT Studies of Conformational Properties of Heteroatom Containing Ketene Analogues and Their Comparison with the Related Cyclic Analogues. <i>E-Journal of Chemistry</i> , 2012 , 9, 193-202		2
23	Ab Initio Study of Conformational Properties of Heteroatom-Containing 1,2-Bis ketene Analogues. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2011 , 186, 1595-1603	1	2
22	Coadsorption of CO and O on H-Capped (6, 0) Single-Walled Carbon Nanotube: A Density Functional Study. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2012 , 20, 233-242	1.8	2
21	Adsorption Properties of H ₂ O ₂ Trapped Inside Boron Nitride Nanotube. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2012 , 20, 243-248	1.8	2
20	Theoretical Study of Cyanate Adsorption on the (6,0) and (7,0) Aluminum Nitride Nanotubes. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2015 , 23, 263-265	1.8	1
19	Electronic and Structural Properties of Ga-Doped (4,4) armchair SiCNT as a p-Semiconductor. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2015 , 23, 54-61	1.8	1
18	Role of Diameter, Model, and Length of Boron Nitride Nanotubes in Adsorption of Formaldehyde. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2015 , 23, 62-67	1.8	1
17	Surface Modification of Carbon Nanotubes with Nitrenes: A DFT Study. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2015 , 23, 326-331	1.8	1
16	Theoretical study of fMet-tRNA and fAla-tRNA structures by using quantum calculation. <i>Arabian Journal of Chemistry</i> , 2016 , 9, S1019-S1028	5.9	1
15	Novel coupling reactions of phytochemicals with sulfa drugs and their applications in the determination of nitrite at trace level in environmental samples. <i>Arabian Journal of Chemistry</i> , 2016 , 9, S812-S820	5.9	1
14	Nanostructures study of chemisorptions of O ₂ molecule on Al (100) surface. <i>Journal of Saudi Chemical Society</i> , 2014 , 18, 469-473	4.3	1

13	Theoretical Study of (CO) n=1, 2 Adsorption on the (6,0) Zigzag Single-walled Carbon Nanotube. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2013 , 21, 117-124	1.8	1
12	Benzene Adsorption on C ₂₄ , Si@C ₂₄ , Si-Doped C ₂₄ , and C ₂₀ Fullerenes. <i>Russian Journal of Physical Chemistry A</i> , 2017 , 91, 2530-2538	0.7	1
11	NMR and NQR study of Si-doped (6,0) zigzag single-walled aluminum nitride nanotube as n or P-semiconductors. <i>Journal of Molecular Modeling</i> , 2012 , 18, 4427-36	2	1
10	Adsorption of sarin and chlorosarin onto the Al ₁₂ N ₁₂ and Al ₁₂ P ₁₂ nanoclusters: DFT and TDDFT calculations. <i>Surface and Interface Analysis</i> , 2020 , 52, 725-734	1.5	1
9	Theoretical Study of Arsenic-Doped (6,0) Zigzag Silicon Carbide Nanotube as a N-Semiconductor. <i>Phosphorus, Sulfur and Silicon and the Related Elements</i> , 2013 , 188, 1382-1393	1	0
8	Adsorption behavior of uracil on external surface of MgO nanotubes: A new class of hybrid nano-bio materials. <i>Journal of Molecular Liquids</i> , 2021 , 339, 116732	6	0
7	Single-Walled Magnesium Oxide Nanotube (6,0) as a Potential Efficient Gas Sensor for HCHO Detection. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2015 , 23, 170-174	1.8	
6	Effect of adsorption sensitivity of armchair single-walled BN nanotube toward thiocyanate anion: A systematic evaluation of length and diameter effects. <i>Surfaces and Interfaces</i> , 2020 , 21, 100693	4.1	
5	Theoretical Study of Single-walled BC ₂ N Nanotubes for Chemical Sensing of Cyanate Ion. <i>Fullerenes Nanotubes and Carbon Nanostructures</i> , 2014 , 22, 789-797	1.8	
4	Magnesium Oxide Nanotube as Potential Sensor for Cl ₂ Detection. <i>Journal of Cluster Science</i> , 2013 , 24, 915-926	3	
3	Adsorption Properties of O ₂ on Cr ₅ Nanostructures: A DFT Study. <i>E-Journal of Chemistry</i> , 2011 , 8, 982-991		
2	Remove of Sulphate Ion from Environmental Systems by using AlN Nanotubes. <i>Bulletin of the Korean Chemical Society</i> , 2014 , 35, 1139-1143	1.2	
1	Production of Pyrimidobenzazepine Derivatives and Reduction of Organic Pollutant Using Ag/Fe ₃ O ₄ /TiO ₂ /CuO@MWCNTs MNCs. <i>Polycyclic Aromatic Compounds</i> , 1-24	1.3	