Mohammad Taghi Baei

List of Publications by Year in Descending Order

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	Ionic liquid as an effective green media for the synthesis of (5Z, 8Z)-7H-pyrido[2,3-d]azepine derivatives and recycable Fe3O4/TiO2/multi-wall cabon nanotubes magnetic nanocomposites as high performance organometallic nanocatalyst. *Molecular Diversity*, **2021**, 1	3.1	3
119	Adsorption behavior of uracil on external surface of MgO nanotubes: A new class of hybrid nano-bio materials. *Journal of Molecular Liquids*, **2021**, 339, 116732	6	0
118	Molecular Modeling and Simulation of glycine functionalized B12N12 and B16N16 nanoclusters as potential inhibitors of proinflammatory cytokines. *Journal of Molecular Liquids*, **2021**, 343, 117494	6	7
117	Effect of adsorption sensitivity of armchair single-walled BN nanotube toward thiocyanate anion: A systematic evaluation of length and diameter effects. *Surfaces and Interfaces*, **2020**, 21, 100693	4.1	
116	Improvement of Antioxidative Activity of Apigenin by B12N12 Nanocluster: Antioxidative Mechanism Analysis. *ChemistrySelect*, **2020**, 5, 1829-1836	1.8	4
115	Influence of the adsorption of toxic agents on the optical and electronic properties of B12N12 fullerene in the presence and absence of an external electric field. *New Journal of Chemistry*, **2020**, 44, 14513-14528	3.6	7
114	Adsorption of sarin and chlorosarin onto the Al12N12 and Al12P12 nanoclusters: DFT and TDDFT calculations. *Surface and Interface Analysis*, **2020**, 52, 725-734	1.5	1
113	A DFT Study on Structure and Electronic Properties of BN Nanostructures Adsorbed with Dopamine. *Computation*, **2019**, 7, 61	2.2	9
112	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. *Heteroatom Chemistry*, **2018**, 29, e21410	1.2	8
111	Structure, stability, and electronic properties of AlP nanocages evolved from the world's smallest caged fullerene C20: A computational study at DFT. *Journal of Molecular Structure*, **2018**, 1159, 118-134	3.4	9
110	Theoretical study on pure and doped B12N12 fullerenes as thiophene sensor. *Adsorption*, **2018**, 24, 585-593	2.3	15
109	Adsorption of chemical warfare agents over C24 fullerene: Effects of decoration of cobalt. *Journal of Alloys and Compounds*, **2018**, 735, 2148-2161	5.7	41
108	A density-functional theory of hydrogen adsorption on indium nitride nanotubes. *Russian Journal of Inorganic Chemistry*, **2017**, 62, 325-335	1.5	4
107	Interaction of pure and metal atom substituted carbon nanocages with CNCl: a DFT study. *Russian Journal of Physical Chemistry B*, **2017**, 11, 354-360	1.2	12
106	Sb(V) removal from copper electrorefining electrolyte: Comparative study by different sorbents. *Transactions of Nonferrous Metals Society of China*, **2017**, 27, 440-449	3.3	15
105	Structural and electronic properties of XY-doped (AlN, AlP, GaN, GaP) C58 fullerenes: a DFT study. *Russian Journal of Inorganic Chemistry*, **2017**, 62, 1067-1076	1.5	5
104	DFT study of the adsorption of H2O2 inside and outside Al12N12 nano-cage. *Russian Journal of Physical Chemistry A*, **2017**, 91, 1527-1534	0.7	7

103	Benzene Adsorption on C24, Si@C24, Si-Doped C24, and C20 Fullerenes. *Russian Journal of Physical Chemistry A*, **2017**, 91, 2530-2538	0.7	1
102	Theoretical study of fMet-tRNA and fAla-tRNA structures by using quantum calculation. *Arabian Journal of Chemistry*, **2016**, 9, S1019-S1028	5.9	1
101	Novel coupling reactions of phytochemicals with sulfa drugs and their applications in the determination of nitrite at trace level in environmental samples. *Arabian Journal of Chemistry*, **2016** , 9, S812-S820	5.9	1
100	Adsorption properties of hydrazine on pristine and Si-doped Al12N12 nano-cage. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2016**, 191, 702-708	1	11
99	BN Nanotube Serving as a Gas Chemical Sensor for N2O by Parallel Electric Field. *Journal of Cluster Science*, **2016**, 27, 1081-1096	3	18
98	Sensitivity of C24 Fullerene to Nicotine Molecule. *Fullerenes Nanotubes and Carbon Nanostructures*, **2015**, 23, 874-877	1.8	6
97	A DFT study of 5-fluorouracil adsorption on the pure and doped BN nanotubes. *Journal of Physics and Chemistry of Solids*, **2015**, 86, 57-64	3.9	48
96	Theoretical Study of Cyanate Adsorption on the (6,0) and (7,0) Aluminum Nitride Nanotubes. *Fullerenes Nanotubes and Carbon Nanostructures*, **2015**, 23, 263-265	1.8	1
95	Electronic and Structural Properties of Ga-Doped (4,4) armchair SiCNT as a p-Semiconductor. *Fullerenes Nanotubes and Carbon Nanostructures*, **2015**, 23, 54-61	1.8	1
94	Role of Diameter, Model, and Length of Boron Nitride Nanotubes in Adsorption of Formaldehyde. *Fullerenes Nanotubes and Carbon Nanostructures*, **2015**, 23, 62-67	1.8	1
93	Al12N12 nanocage as potential adsorbent for removal of acetone from environmental systems. *Monatshefte Fü Chemie*, **2015**, 146, 891-896	1.4	10
92	Surface Modification of Carbon Nanotubes with Nitrenes: A DFT Study. *Fullerenes Nanotubes and Carbon Nanostructures*, **2015**, 23, 326-331	1.8	1
91	Phenol interaction with different nano-cages with and without an electric field: a DFT study. *Structural Chemistry*, **2015**, 26, 685-693	1.8	38
90	C30B15N15 Heterofullerene as a Potential Electronic Sensor for NO Detection. *Fullerenes Nanotubes and Carbon Nanostructures*, **2015**, 23, 153-157	1.8	4
89	Single-Walled Magnesium Oxide Nanotube (6,0) as a Potential Efficient Gas Sensor for HCHO Detection. *Fullerenes Nanotubes and Carbon Nanostructures*, **2015**, 23, 170-174	1.8	
88	Electronic Structure Study of Gallium and Indium Doped (4,4) armchair Single-Walled Boron Nitride Nanotubes for Production of Solid-State Devices. *Fullerenes Nanotubes and Carbon Nanostructures*, **2015**, 23, 68-77	1.8	4
87	A computational study of adenine, uracil, and cytosine adsorption upon AlN and BN nano-cages. *Physica B: Condensed Matter*, **2014**, 444, 6-13	2.8	54
86	Computational study of OCN chemisorption over AlN nanostructures. *Superlattices and Microstructures*, **2014**, 72, 370-382	2.8	8

85	Adsorption phenomena of gas molecules upon Ga-doped BN nanotubes: A DFT study. *Applied Surface Science*, **2014**, 295, 18-25	6.7	25
84	Sensitivity of BN nano-cages to caffeine and nicotine molecules. *Superlattices and Microstructures*, **2014**, 76, 315-325	2.8	65
83	Al12N12 nanocage as a potential sensor for phosgene detection. *Canadian Journal of Chemistry*, **2014**, 92, 605-610	0.9	29
82	The study of SCN adsorption on B 12 N 12 and B 16 N 16 nano-cages. *Superlattices and Microstructures*, **2014**, 75, 716-724	2.8	26
81	Theoretical Study of Single-walled BC2N Nanotubes for Chemical Sensing of Cyanate Ion. *Fullerenes Nanotubes and Carbon Nanostructures*, **2014**, 22, 789-797	1.8	
80	Adsorption of cyanogen chloride over Al- and Ga-doped BN nanotubes. *Superlattices and Microstructures*, **2014**, 75, 564-575	2.8	52
79	Formation and electronic structure of C20 fullerene transition metal clusters. *Monatshefte F Chemie*, **2014**, 145, 1401-1405	1.4	33
78	Adsorption mechanism of single OCN and SCN upon single-walled BP nanotubes. *Physica E: Low-Dimensional Systems and Nanostructures*, **2014**, 59, 66-74	3	10
77	Nanostructures study of chemisorptions of O2 molecule on Al (100) surface. *Journal of Saudi Chemical Society*, **2014**, 18, 469-473	4.3	1
76	Adsorption of the urea molecule on the B$_{12}$N$_{12}$ nanocage. *Turkish Journal of Chemistry*, **2014**, 38, 531-537	1	2
75	Covalent Functionalization of Pristine and Ga-Doped Boron Phosphide Nanotubes with Imidazole. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2014**, 189, 453-464	1	5
74	The electronic and structural properties of BN and BP nano-cages interacting with OCN A DFT study. *Journal of Physics and Chemistry of Solids*, **2014**, 75, 1099-1105	3.9	33
73	Remove of Sulphate Ion from Environmental Systems by using AlN Nanotubes. *Bulletin of the Korean Chemical Society*, **2014**, 35, 1139-1143	1.2	
72	Magnesium Oxide Nanotube as Potential Sensor for Cl2 Detection. *Journal of Cluster Science*, **2013**, 24, 915-926	3	
71	Covalent Functionalization of Zn12O12 Nanocluster with Thiophene. *Journal of Cluster Science*, **2013**, 24, 749-756	3	8
70	First Principles Calculations of Electric Field Effect on the (6,0) Zigzag Single-Walled Silicon Carbide Nanotube for use in Nano-Electronic Circuits. *Journal of Cluster Science*, **2013**, 24, 591-604	3	14
69	Theoretical Study of Phenol Adsorption on Pristine, Ga-Doped, and Pd-Decorated (6,0) Zigzag Single-Walled Boron Phosphide Nanotubes. *Journal of Cluster Science*, **2013**, 24, 49-60	3	16
68	ZnO Nanocluster as a Potential Catalyst for Dissociation of H2S Molecule. *Journal of Cluster Science*, **2013**, 24, 341-347	3	54

67	Transition metal atom adsorptions on a boron nitride nanocage. *Structural Chemistry*, **2013**, 24, 1039-1044	1.8	28
66	Carbon nanocone as an ammonia sensor: DFT studies. *Structural Chemistry*, **2013**, 24, 1099-1103	1.8	58
65	Adsorption and electronic structure study of thiazole on the (6,0) zigzag single-walled boron phosphide nanotube. *Journal of Sulfur Chemistry*, **2013**, 34, 407-420	2.3	8
64	Zn12O12 Fullerene-like Cage as a Potential Sensor for SO2 Detection. *Adsorption Science and Technology*, **2013**, 31, 469-476	3.6	17
63	DFT Study of the Interactions of Carbon Monoxide with Pd-Decorated (6,0) Single-Walled Carbon Nanotube. *Fullerenes Nanotubes and Carbon Nanostructures*, **2013**, 21, 12-18	1.8	3
62	Theoretical Study of (CO) n=1, 2 Adsorption on the (6,0) Zigzag Single-walled Carbon Nanotube. *Fullerenes Nanotubes and Carbon Nanostructures*, **2013**, 21, 117-124	1.8	1
61	Electric field effect on the zigzag (6,0) single-wall BC2N nanotube for use in nano-electronic circuits. *Journal of Molecular Modeling*, **2013**, 19, 97-107	2	11
60	Adsorption of CO molecule on AlN nanotubes by parallel electric field. *Journal of Molecular Modeling*, **2013**, 19, 859-70	2	27
59	Nitrous oxide adsorption on pristine and Si-doped AlN nanotubes. *Journal of Molecular Modeling*, **2013**, 19, 943-9	2	26
58	Covalent functionalization of AlN nanotubes with acetylene. *Physica E: Low-Dimensional Systems and Nanostructures*, **2013**, 47, 147-151	3	8
57	Si-Doped B12N12Nanocage as an Adsorbent for Dissociation of N2O to N2Molecule. *Heteroatom Chemistry*, **2013**, 24, 476-481	1.2	6
56	B12N12 sodalite like cage as potential sensor for hydrogen cyanide. *Computational and Theoretical Chemistry*, **2013**, 1024, 28-33	2	35
55	Selective adsorption behavior of BC2N nanotubes toward fluoride and chloride. *Solid State Communications*, **2013**, 159, 8-12	1.6	20
54	A density functional theory study on acetylene-functionalized BN nanotubes. *Structural Chemistry*, **2013**, 24, 1007-1013	1.8	26
53	Electronic, Energetic, and Geometric Properties of Methylene-Functionalized C60. *Journal of Cluster Science*, **2013**, 24, 669-678	3	12
52	Remove of toxic pyridine from environmental systems by using B12N12 nano-cage. *Superlattices and Microstructures*, **2013**, 58, 31-37	2.8	16
51	Quantum chemical analysis on hydrogenated Zn12O12 nanoclusters. *Comptes Rendus Chimie*, **2013**, 16, 122-128	2.7	19
50	Silicon-doping makes the B12N12 insulator to an n or p-semiconductor. *Superlattices and Microstructures*, **2013**, 60, 437-442	2.8	13

49	Carbon nitride nanotube as a sensor for alkali and alkaline earth cations. *Applied Surface Science*, **2013**, 264, 699-706	6.7	80
48	Fluorination of the exterior surface of AlN nanotube: A DFT study. *Superlattices and Microstructures* , **2013**, 53, 9-15	2.8	19
47	Zn12O12 nano-cage as a promising adsorbent for CS2 capture. *Superlattices and Microstructures*, **2013**, 58, 198-204	2.8	17
46	First-Principles Study of NO2Adsorption on C20Fullerene. *Heteroatom Chemistry*, **2013**, 24, 516-523	1.2	23
45	Adsorption of Thiophene on Aluminum Nitride Nanotubes. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2013**, 188, 1172-1177	1	5
44	Theoretical Study of Arsenic-Doped (6,0) Zigzag Silicon Carbide Nanotube as a N-Semiconductor. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2013**, 188, 1382-1393	1	0
43	DFT Study of CO2Adsorption on the Zn12O12Nano-cage. *Bulletin of the Korean Chemical Society*, **2013**, 34, 3722-3726	1.2	15
42	AlN nanotube as a potential electronic sensor for nitrogen dioxide. *Microelectronics Journal*, **2012**, 43, 452-455	1.8	84
41	Adsorption properties of H2O2 trapped inside a boron phosphide nanotube. *Monatshefte F Chemie*, **2012**, 143, 37-41	1.4	8
40	NMR and NQR parameters of the SiC-doped on the (4,4) armchair single-walled BPNT: a computational study. *Journal of Molecular Modeling*, **2012**, 18, 881-9	2	15
39	Electronic structure study of Si-doped (4,4) armchair single-walled boron phosphide nanotube as a semiconductor. *Monatshefte F Chemie*, **2012**, 143, 1627-1635	1.4	6
38	Electric field effect on (6,0) zigzag single-walled aluminum nitride nanotube. *Journal of Molecular Modeling*, **2012**, 18, 4477-89	2	10
37	NMR and NQR study of Si-doped (6,0) zigzag single-walled aluminum nitride nanotube as n or P-semiconductors. *Journal of Molecular Modeling*, **2012**, 18, 4427-36	2	1
36	Electronic sensor for sulfide dioxide based on AlN nanotubes: a computational study. *Journal of Molecular Modeling*, **2012**, 18, 4745-50	2	70
35	Adsorption of nitrous oxide on the (6,0) magnesium oxide nanotube. *Chinese Chemical Letters*, **2012** , 23, 1275-1278	8.1	15
34	The Al-Doped Carbon Nanotubes: A DFT Study. *Fullerenes Nanotubes and Carbon Nanostructures*, **2012**, 20, 681-687	1.8	15
33	Theoretical study of CO adsorption on the surface of BN, AlN, BP and AlP nanotubes. *Surface Science*, **2012**, 606, 981-985	1.8	125
32	A computational study of AlN nanotube as an oxygen detector. *Chinese Chemical Letters*, **2012**, 23, 965-968	1.8	66

31	Adsorption and Electronic Structure Study of Imidazole on (6,0) Zigzag Single-Walled Boron Nitride Nanotube. *Journal of Cluster Science*, **2012**, 24, 31	3	8
30	Phenol adsorption study on pristine, Ga-, and In-doped (4,4) armchair single-walled boron nitride nanotubes. *Computational and Theoretical Chemistry*, **2012**, 997, 63-69	2	60
29	First-principles calculations of structural stability, electronic, and electrical responses of GeC nanotube under electric field effect for use in nanoelectronic devices. *Superlattices and Microstructures*, **2012**, 52, 1119-1130	2.8	12
28	B-doping makes the carbon nanocones sensitive towards NO molecules. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2012**, 377, 107-111	2.3	79
27	Theoretical study of cyano radical adsorption on (6,0) zigzag single-walled carbon nanotube. *Monatshefte Fü Chemie*, **2012**, 143, 1463-1470	1.4	14
26	Effect of Gallium Doping on Electronic and Structural Properties (6,0) Zigzag Silicon Carbide Nanotube as a p-Semiconductor. *Journal of Cluster Science*, **2012**, 23, 1119-1132	3	16
25	Effects of Zinc Binding on the Structure and Stability of Glycylglycine Dipeptide: A Computational Study. *E-Journal of Chemistry*, **2012**, 9, 1244-1250		6
24	Ab Initioand DFT Studies of Conformational Properties of Heteroatom Containing Ketene Analogues and Their Comparison with the Related Cyclic Analogues. *E-Journal of Chemistry*, **2012**, 9, 193-202		2
23	Co-adsorption of CO molecules at the open ends of MgO nanotubes. *Structural Chemistry*, **2012**, 23, 1981-1986	1.8	18
22	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. *Monatshefte Fü Chemie*, **2012**, 143, 989-995	1.4	5
21	Ge-doped (4,4) armchair single-walled boron phosphide nanotube as a semiconductor: a computational study. *Monatshefte Fü Chemie*, **2012**, 143, 881-889	1.4	6
20	Computational studies on aluminum nitride and aluminum phosphide nanotubes: density functional calculations of 27Al electric field gradient tensors. *Monatshefte Fü Chemie*, **2012**, 143, 545-549	1.4	8
19	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. *Monatshefte Fü Chemie*, **2012**, 143, 1115-1121	1.4	4
18	Coadsorption of CO and O on H-Capped (6, 0) Single-Walled Carbon Nanotube: A Density Functional Study. *Fullerenes Nanotubes and Carbon Nanostructures*, **2012**, 20, 233-242	1.8	2
17	Adsorption Properties of H2O2 Trapped Inside Boron Nitride Nanotube. *Fullerenes Nanotubes and Carbon Nanostructures*, **2012**, 20, 243-248	1.8	2
16	First Principles Study on Encapsulation of Alkali Metals into ZnO Nanocage. *Chinese Journal of Chemical Physics*, **2012**, 25, 671-675	0.9	21
15	Theoretical Study of Thiazole Adsorption on the (6,0) zigzag Single-Walled Boron Nitride Nanotube. *Bulletin of the Korean Chemical Society*, **2012**, 33, 3285-3292	1.2	27
14	A DFT Study on CO2Interaction with a BN Nano-Cage. *Bulletin of the Korean Chemical Society*, **2012**, 33, 3338-3342	1.2	25

13	Adsorption properties of N2O on (6,0), (7,0), and (8,0) zigzag single-walled boron nitride nanotubes: A computational study. *Computational and Theoretical Chemistry*, **2011**, 970, 30-35	2	46
12	The Ge-doped (6,0) zigzag single-walled boron phosphide nanotubes: A computational study. *Computational and Theoretical Chemistry*, **2011**, 972, 14-19	2	14
11	Adsorption Properties of Oxygen onH-Capped (5, 5) Boron Nitride Nanotube (BNNT)- A Density Functional Theory. *E-Journal of Chemistry*, **2011**, 8, 609-614		6
10	Adsorption Properties of O2onCr5Nanostructures: A DFT Study. *E-Journal of Chemistry*, **2011**, 8, 982-991		
9	Adsorption properties of OCN radical on (6,0), (8,0), and (10,0) zigzag single-walled carbon nanotubes: a density functional study. *Monatshefte F□ Chemie*, **2011**, 142, 1-4	1.4	20
8	Adsorption properties of N2O on (6,0), (7,0), (8,0), and Al-doped (6,0) zigzag single-walled carbon nanotubes: a density functional study. *Monatshefte F□ Chemie*, **2011**, 142, 573-578	1.4	14
7	NMR parameters of SiC-doped (6,0) zigzag single-walled boron phosphide nanotubes: a density functional study. *Monatshefte F□ Chemie*, **2011**, 142, 783-788	1.4	10
6	Adsorption properties of SCN□bn (6,0), (7,0), (8,0), and Al-doped (6,0) zigzag single-walled carbon nanotubes: a density functional study. *Monatshefte F□ Chemie*, **2011**, 142, 979-984	1.4	8
5	NMR and NQR parameters of Si-doped (6,0) zigzag single-walled boron phosphide nanotubes: a density functional study. *Monatshefte F□ Chemie*, **2011**, 142, 1097-1104	1.4	12
4	A Dielectric Effect on Normal Mode Analysis and Symmetry of BNNT Nanotube. *Fullerenes Nanotubes and Carbon Nanostructures*, **2011**, 19, 182-196	1.8	4
3	The influence of NH3-attaching on the NMR and NQR parameters in the (6,0) zigzag single-walled BPNTs: a density functional study. *Computational and Theoretical Chemistry*, **2011**, 967, 179-184	2	19
2	Ab Initio Study of Conformational Properties of Heteroatom-Containing 1,2-Bisketene Analogues. *Phosphorus, Sulfur and Silicon and the Related Elements*, **2011**, 186, 1595-1603	1	2
1	Production of Pyrimidobenzazepine Derivatives and Reduction of Organic Pollutant Using Ag/Fe3O4/TiO2/CuO@MWCNTs MNCs. *Polycyclic Aromatic Compounds*,1-24	1.3	