Ali Reza Soltani

List of Publications by Citations

92 papers	1,833 citations	26 h-index	38 g-index
95 ext. papers	2,131 ext. citations	3.8 avg, IF	5.27 L-index

#	Paper	IF	Citations
92	A first-principles study of the adsorption behavior of CO on Al- and Ga-doped single-walled BN nanotubes. *Applied Surface Science*, **2013**, 270, 25-32	6.7	116
91	H2O2 adsorption on the BN and SiC nanotubes: A DFT study. *Physica E: Low-Dimensional Systems and Nanostructures*, **2013**, 48, 176-180	3	100
90	Ab initio investigation of Al- and Ga-doped single-walled boron nitride nanotubes as ammonia sensor. *Applied Surface Science*, **2012**, 263, 619-625	6.7	76
89	Sensitivity of BN nano-cages to caffeine and nicotine molecules. *Superlattices and Microstructures*, **2014**, 76, 315-325	2.8	65
88	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
87	Adsorption of cyanogen chloride over Al- and Ga-doped BN nanotubes. *Superlattices and Microstructures*, **2014**, 75, 564-575	2.8	52
86	Ab initio study of the NO2 and SO2 adsorption on Al12N12 nano-cage sensitized with gallium and magnesium. *Computational Materials Science*, **2013**, 79, 795-803	3.2	51
85	A DFT study on the interaction between 5-fluorouracil and B12N12 nanocluster. *RSC Advances*, **2016**, 6, 104513-104521	3.7	51
84	Adsorption of Celecoxib on BN fullerene: Spectroscopic and DFT/TD-DFT study. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2018**, 204, 348-353	4.4	49
83	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
82	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
81	Electronic and optical properties of 5-AVA-functionalized BN nanoclusters: a DFT study. *New Journal of Chemistry*, **2016**, 40, 7018-7026	3.6	45
80	Adsorption behavior of metformin drug on boron nitride fullerenes: Thermodynamics and DFT studies. *Journal of Molecular Liquids*, **2019**, 275, 955-967	6	45
79	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
78	Ga-doped and antisite double defects enhance the sensitivity of boron nitride nanotubes towards Soman and Chlorosoman. *Applied Surface Science*, **2017**, 411, 1-10	6.7	39
77	Phenol interaction with different nano-cages with and without an electric field: a DFT study. *Structural Chemistry*, **2015**, 26, 685-693	1.8	38
76	Carbon monoxide interactions with pure and doped B11XN12 (X = Mg, Ge, Ga) nano-clusters: a theoretical study. *RSC Advances*, **2015**, 5, 90621-90631	3.7	37

75	Ab initio investigation of the SCN chemisorption of single-walled boron nitride nanotubes. *Applied Surface Science*, **2012**, 258, 9536-9543	6.7	35
74	Interaction of hydrogen with Pd- and co-decorated C24 fullerenes: Density functional theory study. *Synthetic Metals*, **2017**, 234, 1-8	3.6	33
73	Formation and electronic structure of C20 fullerene transition metal clusters. *Monatshefte F Chemie*, **2014**, 145, 1401-1405	1.4	33
72	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
71	Interaction of B12N12 nano-cage with cysteine through various functionalities: A DFT study. *Superlattices and Microstructures*, **2016**, 100, 24-37	2.8	31
70	A first-principles study of functionalized clusters and carbon nanotubes or fullerenes with 5-Aminolevulinic acid as vehicles for drug delivery. *Superlattices and Microstructures*, **2013**, 62, 251-259	2.8	31
69	Al12N12 nanocage as a potential sensor for phosgene detection. *Canadian Journal of Chemistry*, **2014**, 92, 605-610	0.9	29
68	Theoretical investigation of OCN adsorption onto boron nitride nanotubes. *Applied Surface Science*, **2012**, 261, 262-267	6.7	29
67	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
66	Adsorption phenomena of gas molecules upon Ga-doped BN nanotubes: A DFT study. *Applied Surface Science*, **2014**, 295, 18-25	6.7	25
65	Serine adsorption through different functionalities on the BN and Pt-BN nanocages. *Materials Science and Engineering C*, **2018**, 92, 216-227	8.3	25
64	A first-principles study of the SCN chemisorption on the surface of AlN, AlP, and BP nanotubes. *Applied Surface Science*, **2012**, 259, 637-642	6.7	23
63	A comparative theoretical study on the interaction of pure and carbon atom substituted boron nitride fullerenes with ifosfamide drug. *Journal of Molecular Liquids*, **2020**, 297, 111894	6	21
62	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
61	Novel gamma arsenene nanosheets as sensing medium for vomiting agents: A first-principles research. *Computational and Theoretical Chemistry*, **2020**, 1185, 112876	2	19
60	Adsorption and dissociation of H2 on Pd doped graphene-like SiC sheet. *International Journal of Hydrogen Energy*, **2016**, 41, 22886-22898	6.7	19
59	Theoretical studies of hydrazine detection by pure and Al defected MgO nanotubes. *Physica E: Low-Dimensional Systems and Nanostructures*, **2018**, 97, 239-249	3	19
58	Crystal structure, spectroscopic and theoretical studies on two Schiff base compounds of 2,6-dichlorobenzylidene-2,4-dichloroaniline and 2,4-dichlorobenzylidene-2,4-dichloroaniline. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 139, 271-8	4.4	18

57	Gold decorated B12N12 nanocluster as an effective sulfasalazine drug carrier: A theoretical investigation. *Physica E: Low-Dimensional Systems and Nanostructures*, **2020**, 124, 114296	3	18
56	BN Nanotube Serving as a Gas Chemical Sensor for N2O by Parallel Electric Field. *Journal of Cluster Science*, **2016**, 27, 1081-1096	3	18
55	A DFT study of adsorption of glycine onto the surface of BC2N nanotube. *Applied Surface Science*, **2016**, 384, 230-236	6.7	18
54	Preparation, characterization and toxicity evaluation of Co3O4 and NiO-filled multi-walled carbon nanotubes loaded to chitosan. *Nano Structures Nano Objects*, **2017**, 12, 182-187	5.6	16
53	Theoretical study on pure and doped B12N12 fullerenes as thiophene sensor. *Adsorption*, **2018**, 24, 585-593	3.3	15
52	A theoretical study of the adsorption behavior of N2O on single-walled AlN and AlP nanotubes. *Superlattices and Microstructures*, **2013**, 58, 178-190	2.8	15
51	Investigations of adsorption behavior and anti-inflammatory activity of glycine functionalized AlN and AlON fullerene-like cages. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 246, 119023	4.4	15
50	Computational investigation of the electronic and structural properties of CN radical on the pristine and Al-doped (6, 0) BN nanotubes. *Physica B: Condensed Matter*, **2013**, 430, 20-26	2.8	14
49	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 Für Chemie*, **2011**, 142, 573-578	1.4	14
48	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
47	Investigations of adsorption behavior and anti-cancer activity of curcumin on pure and platinum-functionalized B12N12 nanocages. *Journal of Molecular Liquids*, **2021**, 334, 116516	6	12
46	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
45	Synthesis, spectroscopic and photophysical studies of xanthene derivatives. *Journal of Molecular Structure*, **2017**, 1149, 862-873	3.4	11
44	Ab Initio Study of TEPA Adsorption on Pristine, Al and Si Doped Carbon and Boron Nitride Nanotubes. *Journal of Inorganic and Organometallic Polymers and Materials*, **2020**, 30, 4297-4310	3.2	11
43	Al12N12 nanocage as potential adsorbent for removal of acetone from environmental systems. *Monatshefte Für Chemie*, **2015**, 146, 891-896	1.4	10
42	ST8 micellar/niosomal vesicular nanoformulation for delivery of naproxen in cancer cells: Physicochemical characterization and cytotoxicity evaluation. *Journal of Molecular Structure*, **2020**, 1211, 127867	3.4	10
41	Isolation, spectroscopic characterization, X-ray, theoretical studies as well as in vitro cytotoxicity of Samarcandin. *Bioorganic Chemistry*, **2016**, 66, 27-32	5.1	10
40	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

39	A DFT Study on Structure and Electronic Properties of BN Nanostructures Adsorbed with Dopamine. *Computation*, **2019**, 7, 61	2.2	9
38	Adsorption of HCOH and H2S molecules on Al12P12 fullerene: a DFT study. *Adsorption*, **2019**, 25, 235-245	2.6	9
37	Theoretical study of nitrogen, boron, and co-doped (B, N) armchair graphene nanoribbons. *Journal of Molecular Modeling*, **2020**, 26, 64	2	8
36	Computational study of OCN□chemisorption over AlN nanostructures. *Superlattices and Microstructures*, **2014**, 72, 370-382	2.8	8
35	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. *Monatshefte F□ Chemie*, **2011**, 142, 979-984	1.4	8
34	Penicillamine functionalized B12N12 and B12CaN12 nanocages act as potential inhibitors of proinflammatory cytokines: A combined DFT analysis, ADMET and molecular docking study. *Arabian Journal of Chemistry*, **2021**, 14, 103200	5.9	8
33	Interaction of CNCl molecule and single-walled AlN nanotubes using DFT and TD-DFT calculations. *Journal of Saudi Chemical Society*, **2017**, 21, 270-276	4.3	7
32	Effect of the embedded atom on the electronic, optical properties and kinetic stability of [3,6]silaprismane. *Chemical Physics*, **2017**, 487, 59-66	2.3	7
31	Biochemical and biophysical properties of a novel homoisoflavonoid extracted from Scilla persica HAUSSKN. *Bioorganic Chemistry*, **2014**, 57, 51-56	5.1	7
30	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
29	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
28	Cationic vesicles for efficient shRNA transfection in the MCF-7 breast cancer cell line. *International Journal of Nanomedicine*, **2018**, 13, 7107-7121	7.3	7
27	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
26	Non-ionic surfactant vesicles as novel delivery systems for sulfasalazine: Evaluation of the physicochemical and cytotoxic properties. *Journal of Molecular Structure*, **2021**, 1230, 129874	3.4	6
25	Spectroscopic, density functional theory, cytotoxicity and antioxidant activities of sulfasalazine and naproxen drugs combination. *Arabian Journal of Chemistry*, **2021**, 14, 103190	5.9	6
24	A study on the effect of 1-butyl-4-methylpyridinium bromide adsorption on the structural and electronic properties of B12N12 nano-cage. *Journal of Molecular Liquids*, **2019**, 277, 115-122	6	6
23	Predicting adsorption behavior and anti-inflammatory activity of naproxen interacting with pure boron nitride and boron phosphide fullerene-like cages. *Journal of Molecular Liquids*, **2021**, 339, 116678	6	6
22	The interaction of 2,6-dichlorobenzylidene-2,4-dichloroaniline (2,6-DBDA) and 2,4-dichlorobenzylidene-2,4-dichloroaniline (2,4-DBDA) with single-walled carbon nanotube: A DFT study. *Journal of Molecular Structure*, **2016**, 1105, 128-134	3.4	5

21	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
20	Molecular structures, hirshfeld surface analysis, and spectroscopic properties of 6,8-dimethyl-3-(4-chlorophenyl)-7-oxo-7,8-dihydropyrimido[4,5-c]pyridazin-5(6H)-one and 6,8-dimethyl-3-(4-chlorophenyl)-7-thioxo-7,8-dihydropyrimido[4,5-c]pyridazin-5(6H)-one. *Journal of Structural Chemistry*, **2017**, 58, 1332-1340	0.9	5
19	A density-functional theory of hydrogen adsorption on indium nitride nanotubes. *Russian Journal of Inorganic Chemistry*, **2017**, 62, 325-335	1.5	4
18	Antibacterial and Antioxidant Activities and Phytochemical Properties of Punica granatum Flowers in Iran **2018**, 42, 1105-1110		4
17	Crystallography, vibrational, electronic and optical analysis of 4-Bromo-2-(2,5-dichloro-phenylimino)-phenol. *Journal of Molecular Structure*, **2018**, 1173, 521-530	3.4	4
16	A comprehensive spectroscopic, solvatochromic and photochemical analysis of 5-hydroxyquinoline and 8-hydroxyquinoline mono-azo dyes. *Journal of Molecular Structure*, **2021**, 1223, 129323	3.4	4
15	Synthesis, Characterization, Crystal Structure, and DFT Study of 4-Bromo-2-(4,6-Dichloro-Phenylimino)-Phenol. *Journal of Structural Chemistry*, **2019**, 60, 890-897	0.9	3
14	Optical and Electronic Properties of Al-Doped Mg12O12 Nanocluster: A Theoretical Study. *Russian Journal of Inorganic Chemistry*, **2019**, 64, 762-769	1.5	3
13	Kinetic Stability and Reactivity of Silicon and Fluorine-Containing CL-20 Derivatives. *ChemistrySelect* , **2019**, 4, 9659-9665	1.8	3
12	The study of thiazole adsorption upon BC2N nanotube: DFT/TD-DFT investigation. *Structural Chemistry*, **2020**, 31, 1959-1967	1.8	2
11	Electrostatic interaction assisted Ca-decorated C20 fullerene loaded to anti-inflammatory drugs to manage cardiovascular disease risk in rheumatoid arthritis patients. *Journal of Molecular Liquids*, **2022**, 350, 118564	6	2
10	Molecular docking and Density functional theory simulation: Improved anti-inflammatory and anticancer properties of celecoxib using Zinc oxide and magnesium oxide nanoclusters. *Arabian Journal of Chemistry*, **2021**, 103568	5.9	2
9	Sustainable cyanide-C60 fullerene cathode to suppress the lithium polysulfides in a lithium-sulfur battery. *Sustainable Materials and Technologies*, **2022**, 32, e00403	5.3	1
8	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
7	Improved antibacterial activity of sulfasalazine loaded fullerene derivative: computational and experimental studies. *Journal of Molecular Liquids*, **2021**, 118083	6	0
6	Molecular Docking Evaluation of Celecoxib on the Boron Nitride Nanostructures for alleviation of Cardiovascular Risk and inflammatory. *Arabian Journal of Chemistry*, **2021**, 103521	5.9	0
5	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
4	Experimental and theoretical studies of the interaction of Penicillamine with SWCNT (6,0) as a drug delivery system. *Inorganic and Nano-Metal Chemistry*,1-9	1.2	0

3	In vitro release and cytotoxicity study of encapsulated sulfasalazine within LTSP micellar/liposomal and TSP micellar/niosomal nano-formulations. *AEJ - Alexandria Engineering Journal*, **2022**, 61, 9749-9756	6.1	0
2	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	
1	Modeling and simulation of external electric field application for diisopropyl methylphosphonate sensing through B12N12 fullerene. *Journal of Molecular Liquids*, **2021**, 340, 116845	6	