Majid Monajjemi

List of Publications by Year
in descending order

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255	2,532	218592	315616
papers	citations	26	38
		h-index	g-index

267	267	267	1604
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Efficient removal of toxic bromothymol blue and methylene blue from wastewater by polyvinyl alcohol. Journal of Molecular Liquids, 2016, 218, 191-197.	2.3	141
2	The study of adsorption characteristics Cu2+ and Pb2+ ions onto PHEMA and P(MMA-HEMA) surfaces from aqueous single solution. Journal of Hazardous Materials, 2009, 170, 673-679.	6.5	128
3	The Studies of Equilibrium and Thermodynamic Adsorption of Pb(II), Cd(II) and Cu(II) Ions from Aqueous Solution onto SWCNTs and SWCNTâ€“COOH Surfaces. Fullerenes Nanotubes and Carbon Nanostructures, 2010, 18, 285-302.	1.0	123
4	Theoretical Description of Electromagnetic Nonbonded Interactions of Radical, Cationic, and Anionic NH₂BHNBHNH₂ Inside of the B₁₈N₁₈ Nanoring. Journal of Physical Chemistry C, 2010, 114, 15315-15330.	1.5	59
5	Liquid-phase exfoliation (LPE) of graphite towards graphene: An ab initio study. Journal of Molecular Liquids, 2017, 230, 461-472.	2.3	50
6	Theoretical investigation of hydrogen bonding in Watsonâ€“Crick, Hoogestein and their reversed and other models: comparison and analysis for configurations of adenineâ€“thymine base pairs in 9 models. Computational and Theoretical Chemistry, 2005, 714, 43-60.	1.5	43
7	Synthesis of nanocomposites of iron oxide/gold (Fe3O4/Au) loaded on activated carbon and their application in water treatment by using sonochemistry: Optimization study. Ultrasonics Sonochemistry, 2018, 41, 279-287.	3.8	41
8	Quantum investigation of non-bonded interaction between the B15N15 ring and BH2NBH2 (radical,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.0	40
9	A New Generation of B_nN_n Rings as a Supplement to Boron Nitride Tubes and Cages. Journal of Physical Chemistry A, 2013, 117, 1670-1684.	1.1	38
10	Comparison of 4-chloro-2-nitrophenol adsorption on single-walled and multi-walled carbon nanotubes. Iranian Journal of Environmental Health Science & Engineering, 2012, 9, 5.	1.8	36
11	Exchange and Correlation Effect of Hydrogen Chemisorption on Nano V(100) Surface: A DFT Study by Generalized Gradient Approximation (GGA). Journal of Computational and Theoretical Nanoscience, 2011, 8, 763-768.	0.4	33
12	Interaction of Na, Mg, Al, Si with carbon nanotube (CNT): NMR and IR study. Russian Journal of Inorganic Chemistry, 2009, 54, 1465-1473.	0.3	32
13	EPR Study of Electronic Structure of [CoF6]3â^'and B18N18 Nano Ring Field Effects on Octahedral Complex. Journal of Cluster Science, 2011, 22, 673-692.	1.7	32
14	Molecular Modeling Study of Drug-DNA Combined to Single Walled Carbon Nanotube. Journal of Cluster Science, 2012, 23, 259-272.	1.7	32
15	Non bonded interaction between BnNn (stator) and (rotor) systems: A quantum rotation in IR region. Chemical Physics, 2013, 425, 29-45.	0.9	32
16	Computational investigation on alcohol nanosensors in combination with carbon nanotube: a Monte Carlo and ab initio simulation. Ionics, 2013, 19, 155-164.	1.2	32
17	Interaction between threonine and cadmium cation in [Cd(Thr) n]2+ (n = 1â€“3) complexes: density functional calculations. Russian Chemical Bulletin, 2010, 59, 886-889.	0.4	31
18	Alcohol sensors based on SWNT as chemical sensors: Monte Carlo and Langevin dynamics simulation. Microelectronics Journal, 2010, 41, 142-149.	1.1	31

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19	Metal-doped graphene layers composed with boron nitrideâ€“graphene as an insulator: a nano-capacitor. Journal of Molecular Modeling, 2014, 20, 2507.	0.8	30
20	Tin(II)-selective membrane potentiometric sensor using a crown ether as neutral carrier. Sensors and Actuators B: Chemical, 2005, 107, 756-761.	4.0	28
21	Theoretical Investigation of Carbon Nanotube Binding to DNA in View of Drug Delivery. Journal of Computational and Theoretical Nanoscience, 2011, 8, 1212-1219.	0.4	28
22	NMR contour maps as a new parameter of carboxylâ€™s OH groups in amino acids recognition: A reason of tRNAâ€“amino acid conjugation. Chemical Physics, 2014, 433, 1-11.	0.9	28
23	Preparation and characterization of vancomycin-loaded chitosan/PVA/PEG hydrogels for wound dressing. Materials Research Express, 2020, 7, 095401.	0.8	27
24	Investigation of NMR shielding tensors in 1,3 dipolar cycloadditions: solvents dielectric effect. Physics and Chemistry of Liquids, 2008, 46, 299-306.	0.4	26
25	NQR and NMR study of hydrogen bonding interactions in anhydrous and monohydrated guanine cluster model: A computational study. Journal of Structural Chemistry, 2009, 50, 67-77.	0.3	26
26	Solvent Dielectric Effect and Side Chain Mutation on the Structural Stability of Burkholderia cepacia Lipase Active Site: A Quantum Mechanical/Molecular Mechanics Study. Acta Biotheoretica, 2011, 59, 291-312.	0.7	26
27	Theoretical Studies of Solvent Effect on Normal Mode Analysis and Thermodynamic Properties of Zigzag (5, 0) Carbon Nanotube. Fullerenes Nanotubes and Carbon Nanostructures, 2011, 19, 469-482.	1.0	26
28	THE EFFECT OF DIFFERENT SOLVENTS AND TEMPERATURES ON STABILITY OF SINGLE-WALLED CARBON NANOTUBE: A QM/MD STUDY. International Journal of Nanoscience, 2010, 09, 517-529.	0.4	25
29	Simulation of DNA bases in water: Comparison of the Monte Carlo algorithm with molecular mechanics force fields. Biochemistry (Moscow), 2006, 71, S1-S8.	0.7	24
30	Thermochemistry and NBO analysis of peptide bond: Investigation of basis sets and binding energy. Russian Journal of Physical Chemistry A, 2009, 83, 587-597.	0.1	24
31	Theoretical study of solvent effect on NMR shielding tensors of luciferin derivatives. Physics and Chemistry of Liquids, 2011, 49, 561-571.	0.4	24
32	Solvent effects on relative stabilities and 14N NMR shielding of cytosine tautomers: continuous set of gauge transformation calculation using polarizable continuum model. Computational and Theoretical Chemistry, 2002, 581, 51-58.	1.5	23
33	The effects of mono- and divalent metal cations on the solution structure of caffeine and theophylline. Journal of Molecular Structure, 2004, 705, 35-39.	1.8	23
34	A percolation model for carbon nanotube-polymer composites using the Mandelbrot-Given curve. Journal of Structural Chemistry, 2011, 52, 54-59.	0.3	23
35	DFT outlook of solvent effect on function of nano bioorganic drugs. Physics and Chemistry of Liquids, 2012, 50, 596-604.	0.4	23
36	Ionic Strength Dependence of Formation Constants:â€‰ Complexation of Mo(VI) with Aspartic Acid. Journal of Chemical & Engineering Data, 2001, 46, 1140-1144.	1.0	22

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37	Dielectric effect on thermodynamic properties in vinblastine by DFT/Onsager modelling. Physics and Chemistry of Liquids, 2011, 49, 318-336.	0.4	21
38	The pseudo Jahnâ€“Teller effect of puckering in pentatomic unsaturated rings C4AE5, A = N, P, As, E = H, F, Cl. Computational and Theoretical Chemistry, 2015, 1074, 19-25.	1.1	21
39	Thermodynamic study of solvent effects on nanostructures: phosphatidylserine and phosphatidylinositol membranes. Physics and Chemistry of Liquids, 2012, 50, 161-172.	0.4	20
40	Thermodynamic investigation of the ternary mixed electrolyte (CoCl2+ CoSO4+ H2O) system by EMF measurements at T= 298.15 K. Journal of Chemical Thermodynamics, 2010, 42, 1494-1499.	1.0	19
41	A Dielectric Effect on Normal Mode Analysis and Symmetry of BNNT Nanotube. Fullerenes Nanotubes and Carbon Nanostructures, 2011, 19, 182-196.	1.0	19
42	Cell membrane causes the lipid bilayers to behave as variable capacitors: A resonance with self-induction of helical proteins. Biophysical Chemistry, 2015, 207, 114-127.	1.5	19
43	Preparation and characterization of Chicory leaf powder and its application as a nano-native plant sorbent for removal of Acid Blue 25 from aqueous media: isotherm, kinetic and thermodynamic study of the adsorption phenomenon. Journal of Nanostructure in Chemistry, 2020, 10, 75-86.	5.3	19
44	Investigation of Solvent Effects on Armchair Single-Walled Carbon Nanotubes: A QM/MD Study. Fullerenes Nanotubes and Carbon Nanostructures, 2011, 19, 251-261.	1.0	18
45	Monte Carlo simulation study of melittin: Protein folding and temperature dependence. Russian Journal of Physical Chemistry A, 2006, 80, S55-S62.	0.1	17
46	Investigation of different factors towards synthesis of CuS spherical nanoparticles. Journal of Experimental Nanoscience, 2013, 8, 451-461.	1.3	17
47	Nano Theoretical Study of a C₁₆Cluster as a Novel Material for Vitamin C Carrier. Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 687-708.	1.0	17
48	An overview on Coronaviruses family from past to Covid-19: introduce some inhibitors as antiviruses from Gillanâ€™s plants. Biointerface Research in Applied Chemistry, 2020, 10, 5575-5585.	1.0	17
49	Carbazochrome carbon nanotube as drug delivery nanocarrier for anti-bleeding drug: quantum chemical study. Journal of Molecular Modeling, 2022, 28, 11.	0.8	17
50	Metal-stabilized rare tautomers: N4 metalated cytosine (M = Li+, Na+, K+, Rb+ and Cs+), theoretical views. Applied Organometallic Chemistry, 2003, 17, 635-640.	1.7	16
51	Design of fMet-tRNA and Calculation of its Bonding Properties by Quantum Mechanics. Nucleosides, Nucleotides and Nucleic Acids, 2010, 29, 676-683.	0.4	16
52	Ab initio Study of Direct Diffusion Pathway for H⁺, Li⁺, Na⁺, K⁺Cations into the (3,3), (4,4), and (5,5) Open-Ended Single-Walled Carbon Nanotubes. Fullerenes Nanotubes and Carbon Nanostructures, 2012, 20, 163-169.	1.0	16
53	Monte Carlo Quantum Calculation for Double-Walled Carbon Nanotubes (DWNTs) Combined to Calixarene[6]. Journal of Computational and Theoretical Nanoscience, 2013, 10, 2332-2341.	0.4	16
54	Molecular Modeling Investigation of an Anti-cancer Agent Joint to SWCNT Using Theoretical Methods. Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 738-751.	1.0	16

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55	Thermodynamic and Solvent Effect on Dynamic Structures of Nano Bilayer-Cell Membrane: Hydrogen Bonding Study. Journal of Computational and Theoretical Nanoscience, 2015, 12, 3148-3154.	0.4	16
56	Quantum mechanic study of hydrogen chemisorptions on nanocluster vanadium surface. Russian Journal of Inorganic Chemistry, 2008, 53, 1430-1437.	0.3	15
57	Investigation of single wall carbon nanotubes electrical properties and normal mode analysis: Dielectric effects. Russian Journal of Physical Chemistry A, 2009, 83, 2288-2296.	0.1	15
58	Substituent and solvent effects on the structural bioactivity and anticancer characteristic of catechin as a bioactive constituent of green tea. International Journal of Quantum Chemistry, 2011, 111, 2771-2777.	1.0	15
59	Carbon Nanotube as a Deliver for Sulforaphane in Broccoli Vegetable in Point of Nuclear Magnetic Resonance and Natural Bond Orbital Specifications. Journal of Computational and Theoretical Nanoscience, 2014, 11, 1465-1471.	0.4	15
60	Density Functional Theory Study and Anti-Cancer Properties of Shyshaq Plant: In View Point of Nano Biotechnology. Journal of Computational and Theoretical Nanoscience, 2015, 12, 4358-4367.	0.4	15
61	Electron transport phenomenon simulation through the carborane nano-molecular wire. Physica E: Low-Dimensional Systems and Nanostructures, 2008, 40, 2965-2972.	1.3	14
62	Thermodynamic Investigation of Enolâ†"Keto Tautomerism for Alcohol Sensors Based on Carbon Nanotubes as Chemical Sensors. Fullerenes Nanotubes and Carbon Nanostructures, 2010, 18, 45-55.	1.0	14
63	Biophysical chemistry of macrocycles for drug delivery: a theoretical study. Russian Chemical Bulletin, 2011, 60, 238-241.	0.4	14
64	Intermolecular Simulation of Nanobiological Structures in Point of Potential Energy and Second Virial Coefficient. Journal of Computational and Theoretical Nanoscience, 2012, 9, 2208-2214.	0.4	14
65	Theoretical Study of Boron Nitride Nanotubes with Armchair Forms. Fullerenes Nanotubes and Carbon Nanostructures, 2013, 21, 381-393.	1.0	14
66	Theoretical Study of Different Solvent and Temperature Effects on Double-walled Carbon Nanotubes (DWNTs) and Calixarene with Amino Acid: A QM/MM Study. Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 346-361.	1.0	14
67	Harmonic Linear Combination and Normal Mode Analysis of Semiconductor Nanotubes Vibrations. Journal of Computational and Theoretical Nanoscience, 2015, 12, 1030-1039.	0.4	14
68	S-NICS: An Aromaticity Criterion for Nano Molecules. Journal of Computational and Theoretical Nanoscience, 2015, 12, 4895-4914.	0.4	14
69	Sensor Response to Alcohol and Chemical Mechanism of Carbon Nanotube Gas Sensors. Fullerenes Nanotubes and Carbon Nanostructures, 2009, 17, 484-495.	1.0	13
70	Theoretical Study of Different Solvents and Temperatures Effects on Single-Walled Carbon Nanotube and Temozolomide Drug: A QM/MM Study. Fullerenes Nanotubes and Carbon Nanostructures, 2011, 19, 653-667.	1.0	13
71	Amino Functionalized Nano Fe₃O₄@SiO₂ as a Magnetically Green Catalyst for the One-Pot Synthesis of Spirooxindoles Under Mild Conditions. Polycyclic Aromatic Compounds, 2018, 38, 199-212.	1.4	13
72	Preparation, Characterization and First Application of Graphene Oxideâ€Metforminâ€Nickel for the Suzuki Crossâ€Coupling Reaction. ChemistrySelect, 2020, 5, 211-217.	0.7	13

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73	A theoretical thermochemical study of solute-solvent dielectric effects in the displacement of codon-anticodon base pairs. Russian Journal of Physical Chemistry A, 2008, 82, 2277-2285.	0.1	12
74	Non-covalent attraction of B2N(â˜',0) and repulsion of B2N(+) in the B n N n ring: a quantum rotatory due to an external field. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	12
75	Interaction of Tl+3 with mononucleotides: metal ion binding and sugar conformation. Journal of Molecular Structure, 2001, 562, 35-43.	1.8	11
76	NMR shielding and a thermodynamic study of the effect of environmental exposure to petrochemical solvent on DPPC, an important component of lung surfactant. Russian Journal of Physical Chemistry A, 2007, 81, 1956-1963.	0.1	11
77	A DFT study of hydrogen chemisorption on V (100) surfaces. Russian Journal of Physical Chemistry A, 2008, 82, 2354-2361.	0.1	11
78	Vibrational analysis ofp-tert-butyl-calix[4]arene conformers byab initiocalculations. Physics and Chemistry of Liquids, 2008, 46, 379-389.	0.4	11
79	Fractal Dimension on Carbon Nanotube-Polymer Composite Materials Using Percolation Theory. Journal of Computational and Theoretical Nanoscience, 2012, 9, 597-601.	0.4	11
80	(3,3)₄ Armchair Carbon Nanotube in Connection with PNP and NPN Junctions: Ab Initio and DFT-Based Studies. Fullerenes Nanotubes and Carbon Nanostructures, 2013, 21, 213-232.	1.0	11
81	Capacitor simulation including of X-doped graphene (X = Li, Be, B) as two electrodes and (h-BN)_m (m = 1â€“4) as the insulator. Japanese Journal of Applied Physics, 2015, 54, 085101.	0.8	11
82	Evaluation of Coronavirus Families & Covid-19 Proteins: Molecular Modeling Study. Biointerface Research in Applied Chemistry, 2020, 10, 6039-6057.	1.0	11
83	Combined 3D-QSAR modeling and molecular docking study on multi-acting quinazoline derivatives as HER2 kinase inhibitors. EXCLI Journal, 2013, 12, 130-43.	0.5	11
84	Study of the hydrogen bond in different orientations of adenine-thymine base pairs: An ab initio study. Biochemistry (Moscow), 2005, 70, 366-376.	0.7	10
85	Complexation behaviour ofp-t-butyl-calix[4]arene propoxy derivatives toward alkali metal cations in chloroform. Physics and Chemistry of Liquids, 2006, 44, 449-456.	0.4	10
86	Theoretical study of borthiin and its derivatives: structure and aromaticity. Journal of Sulfur Chemistry, 2007, 28, 505-511.	1.0	10
87	Thermodynamic study of interaction of TSPP, CoTsPc, and FeTsPc with calf thymus DNA. Biochemistry (Moscow), 2007, 72, 652-657.	0.7	10
88	Investigation of Langmuir and Freundlich Adsorption Isotherm of Co2+ Ion by Micro Powder of Cedar Leaf. Oriental Journal of Chemistry, 2017, 33, 1569-1574.	0.1	10
89	Theoretical study of the intermolecular potential energy and second virial coefficient in the mixtures of CH₄and Kr gases: a comparison with experimental data. Molecular Simulation, 2010, 36, 865-870.	0.9	9
90	Density Functional Theory Study on B30N20Nanocage in Structural Properties and Thermochemical Outlook. Fullerenes Nanotubes and Carbon Nanostructures, 2013, 21, 503-515.	1.0	9

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91	The Investigation of Sequence-dependent Interaction of Messenger RNA Binding to Carbon Nanotube. Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 643-662.	1.0	9
92	Role of the Salt Bridge Between Arg176 and Glu126 in the Thermal Stability of the Bacillus amyloliquefaciens Î±-Amylase (BAA). Journal of Microbiology and Biotechnology, 2013, 23, 7-14.	0.9	9
93	Thermodynamic Studies on Complexation of Glutamic Acid with Dioxovanadium(V) in Mixed Solvent Systems. Journal of Chemical & Engineering Data, 2001, 46, 1249-1254.	1.0	8
94	QM/MM model study on properties and structure of some antibiotics in gas phase: Comparison of energy and NMR chemical shift. Biochemistry (Moscow), 2006, 71, S113-S122.	0.7	8
95	Charge Density Discrepancy Between NBO and QTAIM in Single-wall Armchair Carbon Nanotubes. Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 575-594.	1.0	8
96	Nano-alumina based (alpha and gamma) drilling fluid system to stabilize high reactive shales. Petroleum, 2021, 7, 142-151.	1.3	8
97	AB INITIO STUDY OF THE INTERACTION OF GUANINE, ADENINE, THYMINE AND CYTOSINE WITH Li+, Na+, Mg2+ AND Sr2+. Main Group Metal Chemistry, 2002, 25, .	0.6	7
98	DFT study of metalâ€“tetrahydroborato ligand interactions in [Ti(CO)4(BH4)]â^'. Computational and Theoretical Chemistry, 2003, 625, 305-314.	1.5	7
99	A Theoretical Study of Metal-Stabilised Rare Tautomers Stability: N4 Metalated Cytosine (M=Be2+,) Tj ETQq1 1 0.784314 rgBT /Overlock 2004, 11-18.	0.6	7
100	An ab initio quantum chemical investigation of solvent-induced effect on 14N-NQR parameters of alanine, glycine, valine, and serine using a polarizable continuum model. Russian Journal of Physical Chemistry A, 2006, 80, S40-S44.	0.1	7
101	Density functional B3LYP and B3PW91 studies of the properties of four cyclic organodiboranes with tetramethylene fragments. Journal of Structural Chemistry, 2010, 51, 437-443.	0.3	7
102	Determination of thermodynamic properties of aqueous mixtures of MgCl2 and Mg(NO3)2 by the potentiometric method at T=298.15. Fluid Phase Equilibria, 2011, 301, 98-104.	1.4	7
103	Non Bonded Interaction of B₁₆N₁₆ Nano Ring with Copper Cations in Point of Crystal Fields. Journal of Computational and Theoretical Nanoscience, 2013, 10, 2473-2477.	0.4	7
104	Interaction of Nano-Boron Nitride/Graphene Sheets with Anode Lithium Ion Battery. Journal of Computational and Theoretical Nanoscience, 2016, 13, 3070-3082.	0.4	7
105	Graphene/(h-BN) n/X-doped graphene as anode material in lithium ion batteries (X=Li, Be, B and N). Macedonian Journal of Chemistry and Chemical Engineering, 2017, 36, 101.	0.2	7
106	Kinetic and Mechanism Studies of the Reaction Between L-Tyrosine and Iodine on the Basis of UV-Vis Spectrophotometric Method. Asian Journal of Biochemistry, 2008, 3, 290-296.	0.5	7
107	Theoretical studies of rotational barriers of dithiocarbamate ligands in the square planar complexes TM(L)(Lâ€²)(H2dtc) (TM=Ir, Rh). Computational and Theoretical Chemistry, 2003, 636, 49-56.	1.5	6
108	Theoretical study of vitamin properties from combined QM-MM methods: Comparison of chemical shifts and energy. Russian Journal of Physical Chemistry A, 2006, 80, 1061-1068.	0.1	6

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109	Thermodynamic Study of the Binding of Mercury Ion to Human Growth Hormone at Different Temperatures. Journal of Solution Chemistry, 2011, 40, 575-586.	0.6	6
110	Study of Bio-nano Interaction Outlook of Amino Acids on Single-walled Carbon Nanotubes. Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 595-603.	1.0	6
111	Symmetry Breaking of B2N(â˜, 0, +): An Aspect of the Electric Potential and Atomic Charges. Molecules, 2015, 20, 21636-21657.	1.7	6
112	Thallium(I) Complexes of Some Sulphur-Containing Ligands. Main Group Metal Chemistry, 2003, 26, 39-48.	0.6	5
113	Complexation of Tri-o-Propoyl-p-t-Butyl Calix[4]Arene with Alkali Metal Cations in Carbon Tetrachloride Solvent. Main Group Metal Chemistry, 2003, 26, .	0.6	5
114	Complexes of Adenine and Guanine with Thallium(I). Main Group Metal Chemistry, 2004, 27, .	0.6	5
115	Thermodynamic Study on the Interaction of Copper Ion with Human Growth Hormone. Journal of Solution Chemistry, 2010, 39, 153-164.	0.6	5
116	Theoretical Studies of Solvent Effects on Binding of Sn (CH3)2(N-acetyl-L-cysteinate) with Single-walled Carbon Nanotube. Fullerenes Nanotubes and Carbon Nanostructures, 2013, 21, 47-63.	1.0	5
117	Quantum Study of Amino Acid Bind to Carbon Nanotube in View of Magnetic Properties. Fullerenes Nanotubes and Carbon Nanostructures, 2014, 22, 709-725.	1.0	5
118	The Double Wall Boron Nitride Nanotube: Nano-Cylindrical Capacitor. Oriental Journal of Chemistry, 2017, 33, 1213-1222.	0.1	5
119	Thermodynamic and IR Spectral Study of Metal Cationsâ€“Anthocyanin Chelation: Mechanism of Formation of Pigments. Russian Journal of Physical Chemistry A, 2020, 94, 1887-1901.	0.1	5
120	The Effect of Exchange and Correlation on Properties of Carbon Nanotube Structure: A DFT study. Journal of the Korean Chemical Society, 2011, 55, 7-13.	0.2	5
121	Removal of Methylene Blue Dye from Aqueous Solutions Using Carboxymethyl-Î²-Cyclodextrin-Fe3O4 Nanocomposite: Thermodynamics andÂKinetics of Adsorption Process. Russian Journal of Physical Chemistry A, 2022, 96, 371-380.	0.1	5
122	Comparison and Thermodynamic Studies on Complexation of Alanine with Vanadium(V) in Mixed Solvent Systems. Journal of Chemical & Engineering Data, 1995, 40, 419-422.	1.0	4
123	A kinetic Monte Carlo simulation study of inositol 1,4,5-trisphosphate receptor (IP3R) calcium release channel. Computational Biology and Chemistry, 2007, 31, 99-109.	1.1	4
124	Density Functional Theory Investigation of Natural Bond Orbital Population Analysis and Gauge-Including Atomic Orbital NMR Tensors of K@B₃₆N₃₆. Journal of Computational and Theoretical Nanoscience, 2010, 7, 1147-1158.	0.4	4
125	Nano theoretical studies of fMet-tRNA structure in protein synthesis of prokaryotes and its comparison with the structure of fAla-tRNA. African Journal of Microbiology Research, 2011, 5, 2667-2674.	0.4	4
126	AIM and NBO analyses on the interaction between SWCNT and cyclophosphamide as an anticancer drug: A density functional theory study. Journal of Theoretical and Computational Chemistry, 2015, 14, 1550021.	1.8	4

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127	Adsorption of Microporous Silica Material (mcm-41) on Graphene Sheet as a Nano-Carrier. Journal of Computational and Theoretical Nanoscience, 2016, 13, 378-387.	0.4	4
128	Neutral Gases Adsorption With Hydrogen on Silicon Nanotubes: A Fuel Cell Invistegation. Oriental Journal of Chemistry, 2017, 33, 1366-1374.	0.1	4
129	Design and Manufacture of Silver-Selective Electrode Based on Single-Walled Carbon Nanotubes. Oriental Journal of Chemistry, 2015, 31, 703-708.	0.1	4
130	A Computational Study of Cytotoxicity of Substituted Amides of Pyrazine- 2-carboxylic acids Using QSAR and DFT Based Molecular Surface Electrostatic Potential. Iranian Journal of Pharmaceutical Research, 2013, 12, 745-50.	0.3	4
131	Complexation of alkali metal ions with di and tri-propyl ether of P-tert-butyl-calix[4]arenes: ab initio approach. Main Group Metal Chemistry, 2004, 27, 107-112.	0.6	3
132	Self-Interaction Error of Local Density Functionals for Molecules and Nanotubes. Fullerenes Nanotubes and Carbon Nanostructures, 2011, 19, 692-699.	1.0	3
133	Solvent effects on tamoxifen molecule interacting with a single-walled carbon nanotube: a theoretical NMR study. Russian Chemical Bulletin, 2012, 61, 2212-2217.	0.4	3
134	DFT Study on 4(5)-Imidazole-carbaldehyde-N(5)-phenylthiosemicarbazone (ImTPh): NMR Shielding Tensors, Thermodynamic Parameters, NBO Analysis, Molecular Electrostatic Potential (MEP), HOMO and LUMO Studies. Oriental Journal of Chemistry, 2014, 30, 345-350.	0.1	3
135	The Electromagnetic Feature of B₁₅N₁₅H_{<I>x</I>} (<I>x</I> = 0, 4, 8, 12, 16, and 20) Nano Rings: Quantum Theory of Atoms in Molecules/NMR Approach. Journal of Computational and Theoretical Nanoscience, 2014, 11, 1290-1298.	0.4	3
136	Electronic Structural Investigation of Boron Nitride Nano Cage (B₃₀N₂₀) in Point of Exchange and Correlation Energy. Journal of Computational and Theoretical Nanoscience, 2015, 12, 652-659.	0.4	3
137	Modeling of Competitive Ultrasonic Assisted Removal of The Crystal Violet and Aura Mineo using Mwcnts Functionalized by N-(3-Nitrobenzylidene)-NĚŠ-Trimethoxysilylpropyl-Ethane-1,2-Diamine:Equilibrium, Kinetics and Thermodynamic Study. Oriental Journal of Chemistry, 2016, 32, 1839-1858.	0.1	3
138	Functionalized Mesoporous Silica Nanoparticle for Levodopa Delivery: A Combination with SWCNTs. Journal of Computational and Theoretical Nanoscience, 2016, 13, 208-219.	0.4	3
139	Adsorption of Thymol Blue and Erythrosine-B on MWCNTs Functionalized by N-(3-nitrobenzylidene)-N'-trimethoxysilylpropyl-ethane-1,2-diamine Equilibrium, Kinetics and Thermodynamic Study. Oriental Journal of Chemistry, 2017, 33, 2542-2550.	0.1	3
140	A review of 2019 fuel cell technologies: modelling and controlling. International Journal of Nanotechnology, 2020, 17, 498.	0.1	3
141	Molecular Dynamic Study of Human Prion Protein upon D178N Mutation: New Perspective to H-bonds, Salt Bridges and the Critical Amino Acids. Protein and Peptide Letters, 2013, 20, 775-780.	0.4	3
142	Novel Auâ€“Fe₃O₄ NPs Loaded on Activated Carbon as a Green and High Efficient Adsorbent for Removal of Dyes from Aqueous Solutions: Application of Ultrasound Wave and Optimization. Eurasian Journal of Analytical Chemistry, 2018, 13, .	0.4	3
143	Bio-Lipid Nano Capacitors: Resonance with Helical Myeline Proteins. Biointerface Research in Applied Chemistry, 2020, 10, 6695-6705.	1.0	3
144	Main Allotropes of Carbon. Advances in Chemical and Materials Engineering Book Series, 2017, , 185-213.	0.2	3

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145	Increasing the efficiency of some antibiotics on penetrating bacteria cell membrane. Ukrainian Journal of Ecology, 2018, 8, 671-679.	0.5	3
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