Afshan Mohajeri

List of Publications by Year
in descending order

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100 papers	1,629 citations	279798 23 h-index	361022 35 g-index
102 all docs	102 docs citations	102 times ranked	2001 citing authors

#	Article	IF	Citations
1	Deep eutecticâ€“water binary solvent associations investigated by vibrational spectroscopy and chemometrics. Physical Chemistry Chemical Physics, 2018, 20, 18463-18473.	2.8	81
2	Theoretical studies on the nature of bonding in Ïƒ-hole complexes. Chemical Physics Letters, 2009, 467, 393-397.	2.6	77
3	Theoretical investigation on antioxidant activity of vitamins and phenolic acids for designing a novel antioxidant. Journal of Molecular Structure, 2009, 930, 15-20.	3.6	70
4	Detection and Evaluation of Hydrogen Bond Strength in Nucleic Acid Base Pairs. Journal of Physical Chemistry A, 2008, 112, 281-295.	2.5	68
5	Fullerene-based materials for solar cell applications: design of novel acceptors for efficient polymer solar cells â€“ a DFT study. Physical Chemistry Chemical Physics, 2015, 17, 22367-22376.	2.8	56
6	Tailoring the optoelectronic properties of graphyne and graphdiyne: nitrogen/sulfur dual doping versus oxygen containing functional groups. Journal of Materials Science, 2017, 52, 5366-5379.	3.7	55
7	Modeling calcium channel antagonistic activity of dihydropyridine derivatives using QTMS indices analyzed by GA-PLS and PC-GA-PLS. Journal of Molecular Graphics and Modelling, 2008, 26, 1057-1065.	2.4	48
8	Edge-functionalized graphene nanoflakes as selective gas sensors. Sensors and Actuators B: Chemical, 2014, 202, 622-630.	7.8	45
9	AIM and NBO analyses of cationâ€“Ï€ interaction. Computational and Theoretical Chemistry, 2006, 774, 71-76.	1.5	42
10	A nano tetraimine Pd(0) complex: synthesis, characterization, computational studies and catalytic applications in the Heckâ€“Mizoroki reaction in water. Green Chemistry, 2015, 17, 3326-3337.	9.0	42
11	Structure and Electronic Properties of Amino Acid Ionic Liquids. Journal of Physical Chemistry A, 2011, 115, 6589-6593.	2.5	41
12	Decorated graphyne and its boron nitride analogue as versatile nanomaterials for CO detection. Molecular Physics, 2015, 113, 3900-3908.	1.7	41
13	Cu2O/TiO2 nanoparticles as visible light photocatalysts concerning C(sp2)â€“P bond formation. Catalysis Science and Technology, 2018, 8, 4044-4051.	4.1	41
14	Halogenâˆ™Hydride Interaction between Zâˆ™X (Z = CN, NC; X = F, Cl, Br) and Hâˆ™Mgâˆ™Y (Y = H, F, Cl, Br,) Tj ETQq0 0 0 rgBT /Overlock 10	2.5	40
15	Aromaticity in terms of ring critical point properties. Chemical Physics Letters, 2008, 458, 378-383.	2.6	36
16	B2-PPW91: A promising double-hybrid density functional for the electric response properties. Journal of Chemical Physics, 2012, 136, 124111.	3.0	30
17	Onicescu information energy in terms of Shannon entropy and Fisher information densities. Molecular Physics, 2012, 110, 403-405.	1.7	30
18	Cooperativity in Bimetallic SACs: An Efficient Strategy for Designing Bifunctional Catalysts for Overall Water Splitting. Journal of Physical Chemistry C, 2019, 123, 30972-30980.	3.1	30

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19	Shannon information entropy of fractional occupation probability as an electron correlation measure in atoms and molecules. Chemical Physics, 2009, 360, 132-136.	1.9	29
20	Density Functional Theory Study on the Static Dipole Polarizability of Boron Nitride Nanotubes: Single Wall and Coaxial Systems. Journal of Physical Chemistry C, 2014, 118, 1739-1745.	3.1	29
21	Computational Insight into the Static and Dynamic Polarizabilities of Aluminum Nanoclusters. Journal of Physical Chemistry A, 2010, 114, 12709-12715.	2.5	28
22	Alizarin red Sâ€“TiO₂-catalyzed cascade C(sp³)â€“H to C(sp²)â€“H bond formation/cyclization reactions toward tetrahydroquinoline derivatives under visible light irradiation. New Journal of Chemistry, 2018, 42, 6880-6888.	2.8	27
23	Application of quantum topological molecular similarity descriptors in QSPR study of the O-methylation of substituted phenols. Journal of Computational Chemistry, 2008, 29, 266-274.	3.3	23
24	Decoration of doped C 60 fullerene with alkali metals: Prototype nanomaterial with enhanced binding energy toward hydrogen. International Journal of Hydrogen Energy, 2017, 42, 12327-12338.	7.1	23
25	Promotional effect of the electron donating functional groups on the gas sensing properties of graphene nanoflakes. RSC Advances, 2015, 5, 54535-54543.	3.6	21
26	Theoretical evidences for resonance-assisted hydrogen bonding. Computational and Theoretical Chemistry, 2004, 678, 201-205.	1.5	20
27	Singlet and triplet potential energy surfaces of C3H2. Computational and Theoretical Chemistry, 2007, 820, 65-73.	1.5	19
28	Light metal decoration on nitrogen/sulfur codoped graphyne: An efficient strategy for designing hydrogen storage media. Physica E: Low-Dimensional Systems and Nanostructures, 2018, 101, 167-173.	2.7	19
29	Molecular designing of triphenylamine-based hole-transporting materials for perovskite solar cells. Solar Energy, 2021, 221, 536-544.	6.1	19
30	Li-decoration on the edge oxidized graphyne and graphdiyne: A first principles study. Computational Materials Science, 2016, 115, 51-59.	3.0	18
31	Ab initio study of multi dihydrogen bonds. Computational and Theoretical Chemistry, 2003, 620, 31-36.	1.5	17
32	The gas-phase acidity and intramolecular hydrogen bonding in oxalic acid. Computational and Theoretical Chemistry, 2004, 711, 167-172.	1.5	17
33	Substituent effect on local aromaticity in mono and diâ€substituted heterocyclic analogs of naphthalene. Journal of Physical Organic Chemistry, 2010, 23, 440-450.	1.9	17
34	Quantitative structure-retention relationship for chromatographic behaviour of anthraquinone derivatives through considering organic modifier features in micellar liquid chromatography. Journal of Chromatography A, 2019, 1599, 46-54.	3.7	17
35	Application of Density Functional Theory for evaluation of standard two-electron reduction potentials in some quinone derivatives. Computational and Theoretical Chemistry, 2008, 870, 10-14.	1.5	16
36	Fine Structural Tuning of Thieno[3,2-b] Pyrrole Donor for Designing Banana-Shaped Semiconductors Relevant to Organic Field Effect Transistors. Journal of Chemical Information and Modeling, 2019, 59, 1930-1945.	5.4	16

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37	Structureâ€“toxicity relationship for aliphatic compounds using quantum topological descriptors. Computational and Theoretical Chemistry, 2008, 855, 1-5.	1.5	15
38	Carbon nanodots as fluorescent platforms for recognition of fluoride ion via the inner filter effect of simple arylboronic acids. Experimental and theoretical investigations. Journal of Fluorine Chemistry, 2016, 190, 12-22.	1.7	15
39	Fe/Nx clusters embedded in graphene with tunable properties for gas separation. Synthetic Metals, 2018, 241, 39-46.	3.9	14
40	Multiâ€way Analysis of Quantum Topological Molecular Similarity Descriptors for Modeling Acidity Constant of Some Phenolic Compounds. Chemical Biology and Drug Design, 2007, 70, 413-423.	3.2	13
41	INFORMATION ENERGY AS AN ELECTRON CORRELATION MEASURE IN ATOMIC AND MOLECULAR SYSTEMS. International Journal of Quantum Information, 2009, 07, 801-809.	1.1	13
42	Aqueous solutions of carbohydrates are new choices of green solvents for highly efficient exfoliation of two-dimensional nanomaterials. Journal of Molecular Liquids, 2020, 309, 113087.	4.9	12
43	Morphological engineering of carbon-based materials: in the quest of efficient catalysts for overall water splitting. International Journal of Hydrogen Energy, 2021, 46, 7284-7296.	7.1	12
44	Molecular Electrostatic Potential as a tool for Evaluating the Etherification Rate Constant. Journal of Physical Chemistry A, 2010, 114, 7417-7422.	2.5	11
45	Impact of position and number of nitrogen atom substitution on the curvature and hydrogen adsorption properties of metallized borophene. Journal of Materials Science, 2018, 53, 4540-4553.	3.7	11
46	Design of nanoscale molecular wire based on diphenylacetylene: Role of linkage. Computational Materials Science, 2009, 45, 935-940.	3.0	10
47	Electron delocalization and aromaticity variations in the stacked nucleic acid base pairs. Structural Chemistry, 2010, 21, 1069-1078.	2.0	10
48	Pi-electron delocalization in aza derivatives of naphthalene and indole. Computational and Theoretical Chemistry, 2011, 976, 19-29.	2.5	10
49	On the relationship between one-electron potential and densities of Fisher information and Shannon entropy. Chemical Physics, 2012, 392, 105-106.	1.9	10
50	Solute-induced perturbation of methanolâ€“water association. RSC Advances, 2015, 5, 71102-71108.	3.6	10
51	EVALUATING THE NATURE OF CHEMICAL BONDS BASED ON PROBABILISTIC MODELS. International Journal of Modern Physics C, 2007, 18, 1795-1809.	1.7	9
52	Kinetic component of the correlation energy density functional: a quantitative description from information theory. Molecular Physics, 2011, 109, 1967-1973.	1.7	9
53	On the optical, electronic, and structural properties of zinc sulfide nanoclusters. International Journal of Quantum Chemistry, 2011, 111, 3841-3850.	2.0	9
54	Zinc selenide nanoclusters: Static dipole polarizability and electronic properties. International Journal of Quantum Chemistry, 2011, 111, 3888-3896.	2.0	9

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55	Global reactivity and site selectivity of (TiO2) nanoclusters (nÂ=Â5â€“10) toward hydrogen peroxide. Materials Chemistry and Physics, 2016, 183, 326-333.	4.0	9
56	The interplay between structural perfectness and CO oxidation catalysis on aluminum, phosphorous and silicon complexes of corroles. Physical Chemistry Chemical Physics, 2019, 21, 7661-7674.	2.8	9
57	METAL ION-LIGAND INTERACTION: HSAB PRINCIPLE VERSUS NBO AND AIM VIEW POINTS. Journal of Theoretical and Computational Chemistry, 2006, 05, 87-98.	1.8	8
58	The role of substituent on the aromaticity variation of mono- and di-substituted aza analogs of indole. Computational and Theoretical Chemistry, 2010, 951, 72-76.	1.5	8
59	On the utility of momentum space in the density functional theory description of the steric effect. Molecular Physics, 2012, 110, 2895-2899.	1.7	8
60	From density functional steric analysis and molecular electrostatic potential to the estimation of etherification rate constant. Journal of Physical Organic Chemistry, 2012, 25, 797-802.	1.9	8
61	Estimation of atomic correlation energies from the electron density at the nucleus and atomic additivity of the correlation energy in molecules. Computational and Theoretical Chemistry, 2009, 907, 115-118.	1.5	7
62	Time-dependent density functional theory benchmarking for the calculations of atomic spectra: efficiency of exc-ETDZ basis set. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	7
63	Assessing the performance of density functional theory for the dynamic polarizabilities of amino acids: Treatment of correlation and role of exact exchange. International Journal of Quantum Chemistry, 2013, 113, 1803-1811.	2.0	7
64	Mg/Cu bimetallic nanoalloys: Morphologies, electronic structures, and catalysis of O2 dissociation. Journal of Alloys and Compounds, 2018, 735, 1962-1970.	5.5	7
65	Catalytic activity of corrole complexes with post-transition elements for the oxidation of carbon monoxide: a first-principles study. New Journal of Chemistry, 2018, 42, 12632-12643.	2.8	7
66	Fine-tuning of charge transport properties of porphyrin donors for organic solar cell. Journal of Molecular Liquids, 2020, 312, 113403.	4.9	7
67	Theoretical study of Diels-Alder reaction: Role of substituent in regioselectivity and aromaticity. Journal of the Iranian Chemical Society, 2010, 7, 554-563.	2.2	6
68	On the performance of density functional schemes for computing the static dipole polarizability of 4d transition-metal monohalides. Molecular Physics, 2011, 109, 1439-1452.	1.7	6
69	Conceptual density functional theory study on dichloropyridines as ambiphilic molecules. Structural Chemistry, 2010, 21, 727-733.	2.0	5
70	A graph theory study on (ZnS)n (n=3â€“10) nanoclusters. Chemical Physics Letters, 2011, 503, 162-166.	2.6	5
71	Nano Structures of Group 13â€“15 Mixed Heptamer Clusters: A Computational Study. Journal of Physical Chemistry A, 2012, 116, 4678-4686.	2.5	5
72	Prediction and characterization of halogenâ€“hydride interaction in Cu n H n Â·Â·Â·ClC2Z and Cu n HÂ·Â·Â·ClC2Z complexes (nÂ=Â2â€“5; ZÂ=ÂH, F, CH3). Structural Chemistry, 2013, 24, 339-348.	2.0	5

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73	Toward More Efficient Organic Semiconductors: The Relationship between Morphology, Charge Transport, and Photophysical Properties. ACS Applied Electronic Materials, 2022, 4, 246-258.	4.3	5
74	Assessment of long-range corrected density functionals for dipole polarizability calculations of MX (M = Y-Cd; X = F, Cl, Br, and I) molecules. Journal of Computational Methods in Sciences and Engineering, 2011, 11, 301-311.	0.2	4
75	Linear optical properties and their bond length dependence of yttrium bromide from ab initio and density functional theory calculations. Chemical Physics, 2011, 387, 5-10.	1.9	4
76	Molecular adsorption of hydrogen peroxide on N- and Fe-doped titania nanoclusters. Applied Surface Science, 2017, 407, 121-129.	6.1	4
77	Endohedral pnicogen and triel bonds in doped C₆₀ fullerenes. New Journal of Chemistry, 2017, 41, 10619-10626.	2.8	4
78	Adsorption of sulfur containing molecules on monoatomic Au, Ag, and binary Au-Ag nanowires: Size and composition dependence. Journal of Alloys and Compounds, 2019, 780, 888-896.	5.5	4
79	In the search of active nanocarriers for delivery of mitomycin C drug. Materials Advances, 2020, 1, 1909-1919.	5.4	4
80	Spin Crossover as an Efficient Strategy for Controllable Gas Molecule Capturing on Open Metal Sites in Ni-BTC and Cu-BTC. Journal of Physical Chemistry C, 2020, 124, 15902-15912.	3.1	4
81	DENSITY FUNCTIONAL THEORY ON FLOATING SPHERICAL GAUSSIAN ORBITAL METHOD. International Journal of Modern Physics C, 2002, 13, 1095-1103.	1.7	3
82	A study of the orbital description of Ï€-bonds in molecules by the FSGO method. Computational and Theoretical Chemistry, 2002, 583, 31-43.	1.5	3
83	Kinetics and Mechanism of the NH (X³Î£^{â€“}) + SO (X³Î£^{â€“}) Reaction: A Theoretical Approach. Journal of Physical Chemistry A, 2020, 124, 6585-6600.	2.5	3
84	Product of position and momentum Fisher information measures under homogeneous potentials. Chemical Physics, 2012, 405, 186-188.	1.9	2
85	Structure and energetics of Li/Na, Li/K, and K/Na bimetallic hexamers. Journal of the Iranian Chemical Society, 2013, 10, 1229-1237.	2.2	2
86	Tuning the halogenâ€“hydride interaction: the role of halogen and metal environments. Molecular Physics, 2015, 113, 463-472.	1.7	2
87	From Subnanometric Clusters toward Single-Atom Catalysts. ACS Symposium Series, 2020, , 17-36.	0.5	2
88	Probing the sensing property of ice nanotubes toward atmospheric gas. Computational and Theoretical Chemistry, 2014, 1038, 49-53.	2.5	1
89	Ammonia nanotubes and their interactions with coinage metals. Chemical Physics, 2014, 441, 159-165.	1.9	1
90	Investigating the nature of intermolecular and intramolecular bonds in noble gas containing molecules. International Journal of Quantum Chemistry, 2015, 115, 165-171.	2.0	1

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91	NO oxidation catalyzed by Ir4-based nanoclusters: the role of alloying on the catalytic activity. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	1
92	Application of chromium-silicon cluster for selective removal of arsenic and sulfide from wastewater. Molecular Physics, 2022, 120, .	1.7	1
93	Ab initio study of three- and five-electron bond molecules, and introducing a new chemical representation. Computational and Theoretical Chemistry, 2002, 588, 155-163.	1.5	0
94	MÃ¸llerâ€“Plesset perturbational self-consistent field theory. Computational and Theoretical Chemistry, 2004, 684, 15-20.	1.5	0
95	On the electronic spectra and optical properties of [(Î·5-C5H5)(L)2M(GaMe2)] complexes (MÂ=ÂFe, Ru, Os;) Tj ETQq1 1 0.784314 rgBT	1.8	0
96	Reply to the â€˜Comment on â€œFullerene-based materials for solar cell applications: design of novel acceptors for efficient polymer solar cells â€“ a DFT studyâ€â€™ by D. S. Sabirov, A. O. Terentyev and I. S. Shepelevich, Phys. Chem. Chem. Phys., 2016, DOI: 10.1039/C5CP05408G. Physical Chemistry Chemical Physics, 2016, 18, 4219-4220.	2.8	0
97	The Evolution of Electronic and Magnetic Properties of the Chain and Sheet Assemblies Based on Planar Tetracoordinate Carbon C₂Al₄(CH₃)₈. Journal of Physical Chemistry A, 2018, 122, 4181-4188.	2.5	0
98	Various Electrode Configurations Effect on the Electronic Transport of CNT/Benzene/CNT System by DFT-NEGF Method. Iranian Journal of Science and Technology, Transaction A: Science, 2021, 45, 1657-1663.	1.5	0
99	Highly Efficient Microwaveâ€assisted Solvent Free Sequantial Oneâ€pot Multicomponent Synthesis of Novel 2â€Hydroxy Indenopyridinâ€5â€ones and Mechanismic Computational Study. Journal of Heterocyclic Chemistry, 0, , .	2.6	0
100	Hydrogen Adsorption on Tiâ€“V Binary and Tiâ€“Vâ€“Al Ternary Alloys of Ti11 Cluster. Journal of Cluster Science, 0, , .	3.3	0