

Afshan Mohajeri

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/4243096/publications.pdf>

Version: 2024-02-01

100
papers

1,629
citations

279487

23
h-index

360668

35
g-index

102
all docs

102
docs citations

102
times ranked

2001
citing authors

#	ARTICLE	IF	CITATIONS
1	Deep eutectic water binary solvent associations investigated by vibrational spectroscopy and chemometrics. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 18463-18473.	1.3	81
2	Theoretical studies on the nature of bonding in π -hole complexes. <i>Chemical Physics Letters</i> , 2009, 467, 393-397.	1.2	77
3	Theoretical investigation on antioxidant activity of vitamins and phenolic acids for designing a novel antioxidant. <i>Journal of Molecular Structure</i> , 2009, 930, 15-20.	1.8	70
4	Detection and Evaluation of Hydrogen Bond Strength in Nucleic Acid Base Pairs. <i>Journal of Physical Chemistry A</i> , 2008, 112, 281-295.	1.1	68
5	Fullerene-based materials for solar cell applications: design of novel acceptors for efficient polymer solar cells – a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 22367-22376.	1.3	56
6	Tailoring the optoelectronic properties of graphyne and graphdiyne: nitrogen/sulfur dual doping versus oxygen containing functional groups. <i>Journal of Materials Science</i> , 2017, 52, 5366-5379.	1.7	55
7	Modeling calcium channel antagonistic activity of dihydropyridine derivatives using QTMS indices analyzed by GA-PLS and PC-GA-PLS. <i>Journal of Molecular Graphics and Modelling</i> , 2008, 26, 1057-1065.	1.3	48
8	Edge-functionalized graphene nanoflakes as selective gas sensors. <i>Sensors and Actuators B: Chemical</i> , 2014, 202, 622-630.	4.0	45
9	AIM and NBO analyses of cation- π interaction. <i>Computational and Theoretical Chemistry</i> , 2006, 774, 71-76.	1.5	42
10	A nano tetraimine Pd(0) complex: synthesis, characterization, computational studies and catalytic applications in the Heck-Mizoroki reaction in water. <i>Green Chemistry</i> , 2015, 17, 3326-3337.	4.6	42
11	Structure and Electronic Properties of Amino Acid Ionic Liquids. <i>Journal of Physical Chemistry A</i> , 2011, 115, 6589-6593.	1.1	41
12	Decorated graphyne and its boron nitride analogue as versatile nanomaterials for CO detection. <i>Molecular Physics</i> , 2015, 113, 3900-3908.	0.8	41
13	Cu ₂ O/TiO ₂ nanoparticles as visible light photocatalysts concerning C(sp ²)-P bond formation. <i>Catalysis Science and Technology</i> , 2018, 8, 4044-4051.	2.1	41
14	Halogen-Hydride Interaction between Z-X (Z = CN, NC; X = F, Cl, Br) and H-Mg-Y (Y = H, F, Cl, Br). <i>Tj ETQq0 Q Q rgBT /Overlock 10</i>	1.1	40
15	Aromaticity in terms of ring critical point properties. <i>Chemical Physics Letters</i> , 2008, 458, 378-383.	1.2	36
16	B2-PPW91: A promising double-hybrid density functional for the electric response properties. <i>Journal of Chemical Physics</i> , 2012, 136, 124111.	1.2	30
17	Onicescu information energy in terms of Shannon entropy and Fisher information densities. <i>Molecular Physics</i> , 2012, 110, 403-405.	0.8	30
18	Cooperativity in Bimetallic SACs: An Efficient Strategy for Designing Bifunctional Catalysts for Overall Water Splitting. <i>Journal of Physical Chemistry C</i> , 2019, 123, 30972-30980.	1.5	30

#	ARTICLE	IF	CITATIONS
19	Shannon information entropy of fractional occupation probability as an electron correlation measure in atoms and molecules. <i>Chemical Physics</i> , 2009, 360, 132-136.	0.9	29
20	Density Functional Theory Study on the Static Dipole Polarizability of Boron Nitride Nanotubes: Single Wall and Coaxial Systems. <i>Journal of Physical Chemistry C</i> , 2014, 118, 1739-1745.	1.5	29
21	Computational Insight into the Static and Dynamic Polarizabilities of Aluminum Nanoclusters. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12709-12715.	1.1	28
22	Alizarin red TiO_2 -catalyzed cascade $\text{C}(\text{sp}^3)\text{H}$ to $\text{C}(\text{sp}^2)\text{H}$ bond formation/cyclization reactions toward tetrahydroquinoline derivatives under visible light irradiation. <i>New Journal of Chemistry</i> , 2018, 42, 6880-6888.	1.4	27
23	Application of quantum topological molecular similarity descriptors in QSPR study of the O-methylation of substituted phenols. <i>Journal of Computational Chemistry</i> , 2008, 29, 266-274.	1.5	23
24	Decoration of doped C 60 fullerene with alkali metals: Prototype nanomaterial with enhanced binding energy toward hydrogen. <i>International Journal of Hydrogen Energy</i> , 2017, 42, 12327-12338.	3.8	23
25	Promotional effect of the electron donating functional groups on the gas sensing properties of graphene nanoflakes. <i>RSC Advances</i> , 2015, 5, 54535-54543.	1.7	21
26	Theoretical evidences for resonance-assisted hydrogen bonding. <i>Computational and Theoretical Chemistry</i> , 2004, 678, 201-205.	1.5	20
27	Singlet and triplet potential energy surfaces of C_3H_2 . <i>Computational and Theoretical Chemistry</i> , 2007, 820, 65-73.	1.5	19
28	Light metal decoration on nitrogen/sulfur codoped graphyne: An efficient strategy for designing hydrogen storage media. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2018, 101, 167-173.	1.3	19
29	Molecular designing of triphenylamine-based hole-transporting materials for perovskite solar cells. <i>Solar Energy</i> , 2021, 221, 536-544.	2.9	19
30	Li-decoration on the edge oxidized graphyne and graphdiyne: A first principles study. <i>Computational Materials Science</i> , 2016, 115, 51-59.	1.4	18
31	Ab initio study of multi dihydrogen bonds. <i>Computational and Theoretical Chemistry</i> , 2003, 620, 31-36.	1.5	17
32	The gas-phase acidity and intramolecular hydrogen bonding in oxalic acid. <i>Computational and Theoretical Chemistry</i> , 2004, 711, 167-172.	1.5	17
33	Substituent effect on local aromaticity in mono and di-substituted heterocyclic analogs of naphthalene. <i>Journal of Physical Organic Chemistry</i> , 2010, 23, 440-450.	0.9	17
34	Quantitative structure-retention relationship for chromatographic behaviour of anthraquinone derivatives through considering organic modifier features in micellar liquid chromatography. <i>Journal of Chromatography A</i> , 2019, 1599, 46-54.	1.8	17
35	Application of Density Functional Theory for evaluation of standard two-electron reduction potentials in some quinone derivatives. <i>Computational and Theoretical Chemistry</i> , 2008, 870, 10-14.	1.5	16
36	Fine Structural Tuning of Thieno[3,2- <i>b</i>] Pyrrole Donor for Designing Banana-Shaped Semiconductors Relevant to Organic Field Effect Transistors. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 1930-1945.	2.5	16

#	ARTICLE	IF	CITATIONS
37	Structure-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.	0.9	15
39	Fe/N _x clusters embedded in graphene with tunable properties for gas separation. Synthetic Metals, 2018, 241, 39-46.	2.1	14
40	Multi-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.	1.5	13
41	INFORMATION ENERGY AS AN ELECTRON CORRELATION MEASURE IN ATOMIC AND MOLECULAR SYSTEMS. International Journal of Quantum Information, 2009, 07, 801-809.	0.6	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.	2.3	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.	3.8	12
44	Molecular Electrostatic Potential as a tool for Evaluating the Etherification Rate Constant. Journal of Physical Chemistry A, 2010, 114, 7417-7422.	1.1	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.	1.7	11
46	Design of nanoscale molecular wire based on diphenylacetylene: Role of linkage. Computational Materials Science, 2009, 45, 935-940.	1.4	10
47	Electron delocalization and aromaticity variations in the stacked nucleic acid base pairs. Structural Chemistry, 2010, 21, 1069-1078.	1.0	10
48	Pi-electron delocalization in aza derivatives of naphthalene and indole. Computational and Theoretical Chemistry, 2011, 976, 19-29.	1.1	10
49	On the relationship between one-electron potential and densities of Fisher information and Shannon entropy. Chemical Physics, 2012, 392, 105-106.	0.9	10
50	Solute-induced perturbation of methanol-water association. RSC Advances, 2015, 5, 71102-71108.	1.7	10
51	EVALUATING THE NATURE OF CHEMICAL BONDS BASED ON PROBABILISTIC MODELS. International Journal of Modern Physics C, 2007, 18, 1795-1809.	0.8	9
52	Kinetic component of the correlation energy density functional: a quantitative description from information theory. Molecular Physics, 2011, 109, 1967-1973.	0.8	9
53	On the optical, electronic, and structural properties of zinc sulfide nanoclusters. International Journal of Quantum Chemistry, 2011, 111, 3841-3850.	1.0	9
54	Zinc selenide nanoclusters: Static dipole polarizability and electronic properties. International Journal of Quantum Chemistry, 2011, 111, 3888-3896.	1.0	9

#	ARTICLE	IF	CITATIONS
55	Global reactivity and site selectivity of (TiO ₂) nanoclusters ($n=5-10$) toward hydrogen peroxide. <i>Materials Chemistry and Physics</i> , 2016, 183, 326-333.	2.0	9
56	The interplay between structural perfectness and CO oxidation catalysis on aluminum, phosphorous and silicon complexes of corroles. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7661-7674.	1.3	9
57	METAL ION-LIGAND INTERACTION: HSAB PRINCIPLE VERSUS NBO AND AIM VIEW POINTS. <i>Journal of Theoretical and Computational Chemistry</i> , 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. <i>Computational and Theoretical Chemistry</i> , 2010, 951, 72-76.	1.5	8
59	On the utility of momentum space in the density functional theory description of the steric effect. <i>Molecular Physics</i> , 2012, 110, 2895-2899.	0.8	8
60	From density functional steric analysis and molecular electrostatic potential to the estimation of etherification rate constant. <i>Journal of Physical Organic Chemistry</i> , 2012, 25, 797-802.	0.9	8
61	Estimation of atomic correlation energies from the electron density at the nucleus and atomic additivity of the correlation energy in molecules. <i>Computational and Theoretical Chemistry</i> , 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. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	7
63	Assessing the performance of density functional theory for the dynamic polarizabilities of amino acids: Treatment of correlation and role of exact exchange. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1803-1811.	1.0	7
64	Mg/Cu bimetallic nanoalloys: Morphologies, electronic structures, and catalysis of O ₂ dissociation. <i>Journal of Alloys and Compounds</i> , 2018, 735, 1962-1970.	2.8	7
65	Catalytic activity of corrole complexes with post-transition elements for the oxidation of carbon monoxide: a first-principles study. <i>New Journal of Chemistry</i> , 2018, 42, 12632-12643.	1.4	7
66	Fine-tuning of charge transport properties of porphyrin donors for organic solar cell. <i>Journal of Molecular Liquids</i> , 2020, 312, 113403.	2.3	7
67	Theoretical study of Diels-Alder reaction: Role of substituent in regioselectivity and aromaticity. <i>Journal of the Iranian Chemical Society</i> , 2010, 7, 554-563.	1.2	6
68	On the performance of density functional schemes for computing the static dipole polarizability of 4d transition-metal monohalides. <i>Molecular Physics</i> , 2011, 109, 1439-1452.	0.8	6
69	Conceptual density functional theory study on dichloropyridines as ambiphilic molecules. <i>Structural Chemistry</i> , 2010, 21, 727-733.	1.0	5
70	A graph theory study on (ZnS) _n ($n=3-10$) nanoclusters. <i>Chemical Physics Letters</i> , 2011, 503, 162-166.	1.2	5
71	Nano Structures of Group 13-15 Mixed Heptamer Clusters: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4678-4686.	1.1	5
72	Prediction and characterization of halogen-hydride interaction in Cu _n H _n and Cu _n H _n Cl ₂ Z and Cu _n H _n Cl ₂ Z complexes ($n=5$; Z=H, F, CH ₃). <i>Structural Chemistry</i> , 2013, 24, 339-348.	1.0	5

#	ARTICLE	IF	CITATIONS
73	Toward More Efficient Organic Semiconductors: The Relationship between Morphology, Charge Transport, and Photophysical Properties. ACS Applied Electronic Materials, 2022, 4, 246-258.	2.0	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.	0.1	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.	0.9	4
76	Molecular adsorption of hydrogen peroxide on N- and Fe-doped titania nanoclusters. Applied Surface Science, 2017, 407, 121-129.	3.1	4
77	Endohedral pnictogen and triel bonds in doped C ₆₀ fullerenes. New Journal of Chemistry, 2017, 41, 10619-10626.	1.4	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.	2.8	4
79	In the search of active nanocarriers for delivery of mitomycin C drug. Materials Advances, 2020, 1, 1909-1919.	2.6	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.	1.5	4
81	DENSITY FUNCTIONAL THEORY ON FLOATING SPHERICAL GAUSSIAN ORBITAL METHOD. International Journal of Modern Physics C, 2002, 13, 1095-1103.	0.8	3
82	A study of the orbital description of π -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(X ³) ⁺ + SO(X ³) ⁺ Reaction: A Theoretical Approach. Journal of Physical Chemistry A, 2020, 124, 6585-6600.	1.1	3
84	Product of position and momentum Fisher information measures under homogeneous potentials. Chemical Physics, 2012, 405, 186-188.	0.9	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.	1.2	2
86	Tuning the halogen-hydride interaction: the role of halogen and metal environments. Molecular Physics, 2015, 113, 463-472.	0.8	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.	1.1	1
89	Ammonia nanotubes and their interactions with coinage metals. Chemical Physics, 2014, 441, 159-165.	0.9	1
90	Investigating the nature of intermolecular and intramolecular bonds in noble gas containing molecules. International Journal of Quantum Chemistry, 2015, 115, 165-171.	1.0	1

#	ARTICLE	IF	CITATIONS
91	NO oxidation catalyzed by Ir ₄ -based nanoclusters: the role of alloying on the catalytic activity. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	1
92	Application of chromium-silicon cluster for selective removal of arsenic and sulfide from wastewater. Molecular Physics, 2022, 120, .	0.8	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	Müller-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 [(η^5 -C ₅ H ₅)(L) ₂ M(GaMe ₂)] complexes (M=Fe, Ru, Os; L=EtO, 1,1,0.784314 rg	0.8	0
96	Reply to the "Comment on "Fullerene-based materials for solar cell applications: design of novel acceptors for efficient polymer solar cells" a DFT study" 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.	1.3	0
97	The Evolution of Electronic and Magnetic Properties of the Chain and Sheet Assemblies Based on Planar Tetracoordinate Carbon C ₂ Al ₄ (CH ₃) ₈ . Journal of Physical Chemistry A, 2018, 122, 4181-4188.	1.1	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.	0.7	0
99	Highly Efficient Microwave-assisted Solvent Free Sequential One-pot Multicomponent Synthesis of Novel 2-Hydroxy Indenopyridinones and Mechanistic Computational Study. Journal of Heterocyclic Chemistry, 0, , .	1.4	0
100	Hydrogen Adsorption on Ti-V Binary and Ti-V-Al Ternary Alloys of Ti ₁₁ Cluster. Journal of Cluster Science, 0, , .	1.7	0