Hossein Roohi

List of Publications by Year
in descending order

90	998	567281 15	580821 25
papers	citations	h-index	g-index

90	90	90	999
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quantum chemical studies on nanostructures of the hydrated methylimidazoliumâ€“based ionic liquids. Journal of Molecular Modeling, 2015, 21, 1.	1.8	96
2	H-bonded complexes of uracil with parent nitrosamine: A quantum chemical study. Computational and Theoretical Chemistry, 2011, 965, 211-220.	2.5	82
3	Excited state intramolecular proton transfer (ESIPT) in 2-(2â€²-hydroxyphenyl)benzoxazole and its naphthalene-fused analogs: A TD-DFT quantum chemical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 118, 228-238.	3.9	46
4	Anomeric effect and rotational barrier in fluoromethanol: A theoretical study. Computational and Theoretical Chemistry, 2005, 726, 141-148.	1.5	30
5	Ion-pairs formed in [Mim+][N(CN)2â^] ionic liquid: Structures, binding energies, NMR SSCCs, volumetric, thermodynamic and topological properties. Journal of Molecular Liquids, 2013, 177, 119-128.	4.9	29
6	Intramolecular photoinduced proton transfer in 2-(2â€²-hydroxyphenyl)benzazole family: A TD-DFT quantum chemical study. Chemical Physics, 2014, 444, 66-76.	1.9	22
7	Effect of the Stoneâ€“Wales (SW) defect on the response of BNNT to axial tension and compression: a quantum chemical study. Structural Chemistry, 2015, 26, 11-22.	2.0	22
8	Influence of various anions and cations on electrochemical and physicochemical properties of the nanostructured Tunable Aryl Alkyl Ionic Liquids (TAAILs): A DFT M06-2X study. Thermochimica Acta, 2016, 639, 20-40.	2.7	20
9	Hydrogen bonding in acetylacetaldehyde: Theoretical insights from the theory of atoms in molecules. International Journal of Quantum Chemistry, 2009, 109, 1505-1514.	2.0	19
10	Molecular interactions in methylimidazolium tetrafluoroborate ionic liquid ([Mim+][BF4â^]): Structures, binding energies, topological properties and NMR one- and two bonds spinâ€“spin coupling constants. Journal of Molecular Liquids, 2011, 161, 63-71.	4.9	19
11	The role of the donor group and electron-accepting substitutions inserted in Ï€-linkers in tuning the optoelectronic properties of Dâ€“Ï€â€“A dye-sensitized solar cells: a DFT/TDDFT study. RSC Advances, 2022, 12, 11557-11573.	3.6	19
12	Exploring the adsorption of CO toxic gas on pristine and M-doped (M = Ti, Cr, Fe, Ni and Zn) GaN nanosheets. New Journal of Chemistry, 2019, 43, 15280-15292.	2.8	18
13	Exploring physicochemical properties of the nanostructured Tunable Aryl Alkyl Ionic Liquids (TAAILs). Journal of Molecular Liquids, 2015, 209, 14-24.	4.9	17
14	Quantum mechanical study of tautomerism of methimazole and the stability of methimazoleâ€“I2 complexes. Computational and Theoretical Chemistry, 2004, 710, 77-84.	1.5	16
15	The gas phase hydrogen-bonded dimers of HOCl: A high-level quantum chemical study. International Journal of Quantum Chemistry, 2010, 110, 1489-1499.	2.0	16
16	AIM and NBO analyses of Nâ€“N rotational barrier in monocyclic nitrosamine compounds. Chemical Physics Letters, 2005, 409, 212-218.	2.6	15
17	Influence of substitution on the strength and nature of CHÂ·Â·Â·N hydrogen bond in XCCHÂ·Â·Â·NH₃complexes. International Journal of Quantum Chemistry, 2011, 111, 961-969.	2.0	15
18	Photo-induced proton transfer in fluorene- and carbazole-based compounds as red- and orange-light-emitting molecules: A TD-DFT study. Organic Electronics, 2015, 25, 121-130.	2.6	15

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19	Restricted rotation in five-membered cyclic nitrosamine compounds: DFT investigation of structural, energetic and kinetics properties. Computational and Theoretical Chemistry, 2001, 543, 299-308.	1.5	14
20	Proton transfer from H2O to p-substituted anilide anion: can the size of water cluster influence the N-â‹…â‹…â‹…Hâ€“OHâ†'Nâ€“Hâ‹…â‹…â‹…OH- switching. Journal of Molecular Modeling, 2012, 18, 1313-1324.	1.8	14
21	Influence of functionalized multi-layer graphene on adhesion improvement and corrosion resistance performance of zinc-rich epoxy primer. Corrosion Engineering Science and Technology, 2018, 53, 422-430.	1.4	14
22	Experimental and DFT mechanistic insights into one-pot synthesis of 1H-pyrazolo[1,2-b]phthalazine-5,10-diones under catalysis of DBU-based ionic liquids. New Journal of Chemistry, 2020, 44, 16594-16601.	2.8	14
23	Adsorption behaviour of NO, NO2, CO and CS2 molecules on the surface of carbon-doped gallium nitride nanosheet: A DFT study. Surface Science, 2022, 717, 121988.	1.9	14
24	Green chemical functionalization of single-wall carbon nanotube with methylimidazolium dicyanamid ionic liquid: A first principle computational exploration. Journal of Molecular Liquids, 2015, 211, 498-505.	4.9	13
25	Tuning the structural, electronic and electrochemical properties of the 4-methyl-1-phenyl triazolium based [PhMeTAZ][Y 1â€“8] ionic liquids through changing anions: A quantum chemical study. Journal of Molecular Liquids, 2017, 240, 138-151.	4.9	13
26	Non-covalent green functionalization of boron nitride nanotubes with tunable aryl alkyl ionic liquids: A quantum chemical approach. Journal of Molecular Liquids, 2017, 243, 22-40.	4.9	13
27	NBO and AIM analyses of the anomeric effect in fluoromethanthiol. Computational and Theoretical Chemistry, 2006, 772, 65-73.	1.5	12
28	Interaction between O3 and H2O2: A theoretical study. Chemical Physics Letters, 2008, 460, 72-78.	2.6	12
29	Effect of axial strain on structural and electronic properties of zig-zag type of boron nitride nanotube (BNNT): a quantum chemical study. Structural Chemistry, 2013, 24, 409-420.	2.0	12
30	Experimental and theoretical probing of the physicochemical properties of ionic liquids composed of [Bn-DBU]+ cation and various anions. Journal of Molecular Structure, 2020, 1202, 127226.	3.6	12
31	Substituent effects on the halogen and pnictogen bonds characteristics in ternary complexes 4-YPhNH2Â·Â·Â·PH2FÂ·Â·Â·ClX (Yâ€‰=â€‰H, F, CN, CHO, NH2, CH3, NO2 and OCH3, and Xâ€‰=â€‰F, OH, CN, NC, FCC and NO2): theoretical study. Journal of Chemical Sciences, 2020, 132, 1.	1.5	11
32	Theoretical investigation of nitric oxide adsorption on the surface of pure and metal (Ti, Cr, Fe, Ni and) Tj ETQq0 0 0 rgBT /Overlock 10 T 120, 114075.	2.7	11
33	DFT study of the biphenyleneâ€“NO complexes formed in nitration mechanism. Journal of Physical Organic Chemistry, 2008, 21, 971-978.	1.9	10
34	Atomic and electronic structures of finite single-walled BN nanotubes: Hybrid DFT calculations. Computational and Theoretical Chemistry, 2008, 856, 46-58.	1.5	10
35	Adsorption of parent nitrosamine on the nanocrystaline Hâ€“zeolite: A theoretical study. Applied Surface Science, 2010, 256, 7575-7582.	6.1	10
36	Chemical functionalization of boron nitride nanotube via the 1,3-dipolar cycloaddition reaction of azomethine ylide: a quantum chemical study. Structural Chemistry, 2015, 26, 749-759.	2.0	10

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37	Photoswitching in nanostructured benzofuro[3,2- b]pyridin-9-ol and benzothio[3,2- b] pyridin-9-ol compounds as red- and yellow-light-emitting molecules: A TD-DFT approach. Dyes and Pigments, 2016, 134, 106-117.	3.7	10
38	Effect of CH3CO functional group on the molecular and electronic properties of BN43zz nanotube: A computational chemistry study. Computational and Theoretical Chemistry, 2010, 952, 36-45.	1.5	9
39	Intra-cluster proton transfer in anilideâ€“(HF)n (n=1â€“4): Can the size of HF cluster influence the Nâˆ’â‹¯Hâ€“Fâ†’Nâ€“Hâ‹¯Fâˆ’ switching. Journal of Fluorine Chemistry, 2011, 132, 459-467.	1.7	9
40	Fine tuning the emission wavelengths of the 7-hydroxy-1-indanone based nano-structure dyes: Near-infrared (NIR) dual emission generation with large stokes shifts. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 196, 83-102.	3.9	9
41	Physicochemical properties of the imidazolium-based dicationic ionic liquids (DILs) composed of ethylene Ï€-spacer by changing the anions: a quantum chemical approach. Ionics, 2020, 26, 1963-1988.	2.4	9
42	Adsorption performance of M-doped (M = Ti and Cr) gallium nitride nanosheets towards SO₂ and NO₂: a DFT-D calculation. RSC Advances, 2020, 10, 27805-27814.	3.6	9
43	Tuning the electronic properties of SiC nanosheets decorated by Lin (nâ€‰=â€‰1â€“3) for the anode of lithium-ion batteries. Molecular Physics, 2020, 118, e1786182.	1.7	9
44	DFT, AIM, and NBO analyses of 1-methyl-2-thioxoimidazolidin-4-one tautomers and their complexes with iodine. Journal of Structural Chemistry, 2012, 53, 649-658.	1.0	8
45	NMR chemical shielding and spinâ€“spin coupling constants across hydrogen bonds in uracilâ€“Î±-hydroxy-N-nitrosamine complexes. Structural Chemistry, 2014, 25, 483-493.	2.0	8
46	Exploring the physicochemical properties of para-xylyl linked DBU-based dicationic ionic liquids consist of various anions: A GD3â€“M06â€“2X study. Journal of Molecular Liquids, 2020, 310, 113060.	4.9	8
47	Proton-Transfer Mechanism in 2-Thioxoimidazolidin-4-one: A Competition between Keto/Enol and Thione/Thiol Tautomerism Reactions. Bulletin of the Chemical Society of Japan, 2009, 82, 446-452.	3.2	7
48	Nï£¿HÂ·Â·Â·S and Sï£¿HÂ·Â·Â·N intramolecular hydrogen bond in Î²â€thioaminoacrolein: A quantum chemical study. International Journal of Quantum Chemistry, 2011, 111, 3008-3016.	2.0	7
49	Noncatalytic Liquid Phase Air Oxidation of Ethylbenzene to 1-Phenyl Ethyl Hydroperoxide in Low Oxygen Volume Fraction. Organic Process Research and Development, 2018, 22, 136-146.	2.7	7
50	Molecular engineering of the photo switching in the ortho chromophores of the nanostructured green fluorescence protein. Journal of Luminescence, 2018, 196, 406-424.	3.1	7
51	Mechanism of the photo triggered ring-opening reaction of spiropyran derivatives (SP-X1-7; X1-7 = H,) Tj ETQq1 1 0.784314 rgBT /Ov Journal of Photochemistry and Photobiology A: Chemistry, 2020, 392, 112410.	3.9	7
52	Methimazole-disulfide as an Anti-Thyroid Drug Metabolite Catalyzed the Highly Regioselective Conversion of Epoxides to Halohydrins with Elemental Halogens. Bulletin of the Korean Chemical Society, 2008, 29, 51-56.	1.9	7
53	Conformations of O3â€“F 1:1 Complexes. An Ab Initio Study. Bulletin of the Chemical Society of Japan, 2007, 80, 1914-1919.	3.2	6
54	Adsorption of methanol on the nanocrystalline Hâ€“zeolite and alkali metal exchanged Mâ€“zeolites: Energetic, NBO and QTAIM analyses. Microporous and Mesoporous Materials, 2008, 113, 240-251.	4.4	6

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55	Quantum chemical study of the O3â€“HONO complex. Chemical Physics Letters, 2009, 476, 168-173.	2.6	6
56	Can the substituent in the para position of anilide ion influence the Nâ^'Â·Â·Â·Hâ€“FÂâ†'ÂNâ€“HÂ·Â·Â·Fâ^' switching; a quantum chemical study. Structural Chemistry, 2013, 24, 1319-1330.	2.0	6
57	Effects of C1â€“3-doping on electronic and structural properties of Stoneâ€“Wales defective boron nitride nanotubes as well as their NO gas sensitivity. RSC Advances, 2016, 6, 11353-11369.	3.6	6
58	Practical one-pot synthesis of semicarbazone derivatives via semicarbazide, and evaluation of their antibacterial activity. Research on Chemical Intermediates, 2016, 42, 3625-3636.	2.7	6
59	Exploring electronic properties and NO gas sensitivity of Si-doped SW-BNNTs under axial tensile strain. Journal of Materials Science, 2017, 52, 9739-9763.	3.7	6
60	Molecular engineering of the electronic, structural, and electrochemical properties of nanostructured 1-methyl-4-phenyl 1,2,4 triazolium-based [PhMTZ][X1â€“10] ionic liquids through anionic changing. Ionics, 2018, 24, 483-504.	2.4	6
61	Fine-tuned dual fluorescence behavior of N-substituted aniline-imidazopyridine based switches: Mechanistic understanding, substituent and solvent effects. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 214, 407-428.	3.9	6
62	Topological and natural population analyses of gas-phase identity SN2 reactions of some methyl halides: Backside attack. Chemical Physics Letters, 2006, 419, 179-183.	2.6	5
63	Effect of Hydration and Self-Association on the Reaction Mechanism of Proton Transfer in Methimazole: A Theoretical Study. Bulletin of the Chemical Society of Japan, 2008, 81, 1402-1414.	3.2	5
64	Iodometric Determination of Hydroperoxides in Hydrocarbon Autoxidation Reactions Using Triphenylphosphine Solution as a Titrant: A New Protocol. Industrial & Engineering Chemistry Research, 2018, 57, 6805-6814.	3.7	5
65	Adsorption of cytarabine and gemcitabine anticancer drugs on the BNNT surface: DFT and GD3-DFT approaches. Adsorption, 2020, 26, 1365-1384.	3.0	5
66	Exploring the electrochemical windows of Triazolium-based [PhMTZ][X1â€“7] ionic liquids (ILs) at MP2/Aug-cc-pVDZ level of theory by using thermochemical cycle in IL media. Journal of Electroanalytical Chemistry, 2020, 877, 114606.	3.8	5
67	Characterization of the Nï£¿HÂ·Â·Â·Oï£¾N and Nï£¿HÂ·Â·Â·Nï£¾O Hâ€bonds in nitrosamine dimers. International Journal of Quantum Chemistry, 2008, 108, 462-471.	2.0	4
68	Interaction between NH₂NO and H₂O₂: A quantum chemistry study. International Journal of Quantum Chemistry, 2010, 110, 1972-1981.	2.0	4
69	Conformational and tautomeric preferences in 3â€aminoacrylaldehyde: A theoretical study. International Journal of Quantum Chemistry, 2011, 111, 586-595.	2.0	4
70	Thermodynamic and topological investigation of the interaction between methimazole and Mz+ (Na+,) Tj ETQq0 0 0 rgBT /Overlock 10 T	2.5	4
71	Generalized Anomeric Effect in CH4â^'nClnS. Energetic and NBO Analyses. Bulletin of the Chemical Society of Japan, 2007, 80, 1323-1330.	3.2	3
72	Theoretical study of solvent effects on the conformational preference in CH2FWH (W=O, S) using PCM and IPCM methods. Journal of Molecular Liquids, 2008, 143, 119-124.	4.9	3

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73	Adsorption of parent nitrosamine on the nanocrystaline M-ZSM-5 zeolite: A density functional study. Journal of Chemical Sciences, 2013, 125, 1607-1618.	1.5	3
74	Quantum chemical study of the interaction between selenium analog of methimazole as an anti-thyroid drug and metal cations. Structural Chemistry, 2014, 25, 1635-1645.	2.0	3
75	Exploring the pnicogen bond non-covalent interactions in 4-XPhNH2:PFnH3-n complexes (n = 1â€“3, X = H,) Tj ETQq1 1 0.784314 rgBT	1.7	3
76	Computational evidence of new putative allosteric sites in the acetylcholinesterase receptor. Journal of Molecular Graphics and Modelling, 2021, 107, 107981.	2.4	3
77	Blue-shifted H-bond in aromatic sulfines: An ab initio calculation. International Journal of Quantum Chemistry, 2007, 107, 1559-1565.	2.0	2
78	Influence of hydration on the protomeric tautomerism in selenium analogue of methimazole: A computational chemistry study. Computational and Theoretical Chemistry, 2009, 910, 41-49.	1.5	2
79	Influence of axial tensile strain on the electronic and structural properties as well as NO gas sensitivity and reactivity of C-doped SW-BNNTs. Surface Science, 2017, 665, 62-82.	1.9	2
80	Fine-tuning the photophysical properties of the five quinolin based nanophotoswitches in the gas phase, polar and nonpolar solvents: A TD-DFT approach. Journal of Luminescence, 2018, 204, 230-243.	3.1	2
81	Decomposition mechanism of the phenylaminyl C6H5N H radical to propargyl and acetylene: A M06-2X, CBS-QB3 and G4 study. Chemical Physics Letters, 2019, 730, 332-339.	2.6	2
82	Tuning the physicochemical properties of the single-walled boron nitride nanotube by covalent grafting of triazolium-based [MTZ][X1â€“3] (X1â€“3= NTf2â^', TfOâ^' and BF4â^') ionic liquids in the gas phase and solvent media: A quantum chemical approach. Journal of Molecular Liquids, 2019, 277, 726-737.	4.9	2
83	Molecular engineering of the efficiency of new thieno[3,2-b]thiophene-based metal-free dyes owning different donor and Ï€-linkers groups for use in the dye-sensitised solar cells: a quantum chemical study. Molecular Physics, 2021, 119, e1913250.	1.7	2
84	Synthesis and characterization of dicationic and monocationic fluorine-containing DBU based ionic liquids: Experimental and quantum chemical approaches. Journal of Molecular Structure, 2021, 1245, 131123.	3.6	2
85	Evaluation of the origin of rotational barrier in NH2X (X=NO, NS). Computational and Theoretical Chemistry, 2006, 778, 63-67.	1.5	1
86	The quantum chemical calculation of NMR two-bond spinâ€“spin coupling constants in the Nâ^'Â·Â·Â·Hâ€“OHÂâ†'ÂNâ€“HÂ·Â·Â·OHâ^' switching. Structural Chemistry, 2012, 23, 825-830.	2.0	1
87	Adsorption sensitivity of nanocrystalline B-substituted H-ZSM-5 and alkali metal-exchanged M-ZSM-5 zeolites towards parent nitrosamine: A B97D study. Computational and Theoretical Chemistry, 2015, 1066, 76-87.	2.5	1
88	Adsorption performance of TM doped (TMâ€‰=â€‰Fe, Ni, Cr and Zn) silicon carbide nanotubes towards formaldehyde: a DFT-M06-L study. Molecular Physics, 0, , .	1.7	1
89	Influence of HOClâ€¦O₃and HOClâ€¦HOCl interactions on the stability of O₃(HOCl)₂complexes: a theoretical study. Molecular Simulation, 2011, 37, 386-393.	2.0	0
90	The interplay between anion-Ï€ and H-bonding interactions in Xâ^'Â·Â·Â·s-TriazineÂ·Â·Â·(HF)n(HCl)3-n (Xâ€‰=â€‰Fâ^', Clâ^') Tj ETQq0 0	1.7	0