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	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
2	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
3	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€‰F, Clâ^') Tj ETQq	1.7	0
4	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
5	Computational evidence of new putative allosteric sites in the acetylcholinesterase receptor. Journal of Molecular Graphics and Modelling, 2021, 107, 107981.	2.4	3
6	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
7	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
8	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
9	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
10	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
11	Adsorption of cytarabine and gemcitabine anticancer drugs on the BNNT surface: DFT and GD3-DFT approaches. Adsorption, 2020, 26, 1365-1384.	3.0	5
12	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
13	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
14	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
15	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
16	Mechanism of the photo triggered ring-opening reaction of spiropyran derivatives (SP-X1-7; X1-7 = H,) Tj ETQq0 0 0 rgBT /Overlock 10 T Journal of Photochemistry and Photobiology A: Chemistry, 2020, 392, 112410.	3.9	7
17	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
18	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

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19	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
20	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
21	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
22	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
23	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
24	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
25	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
26	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
27	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
28	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
29	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
30	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
31	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
32	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
33	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
34	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
35	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
36	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

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37	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
38	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
39	Quantum chemical studies on nanostructures of the hydrated methylimidazoliumâ€“based ionic liquids. Journal of Molecular Modeling, 2015, 21, 1.	1.8	96
40	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
41	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
42	Exploring physicochemical properties of the nanostructured Tunable Aryl Alkyl Ionic Liquids (TAAILs). Journal of Molecular Liquids, 2015, 209, 14-24.	4.9	17
43	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
44	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
45	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
46	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
47	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
48	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
49	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
50	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
51	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
52	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
53	Thermodynamic and topological investigation of the interaction between methimazole and Mz+ (Na+,) Tj ETQq1 1 0.784314 rgBT /Ov	2.5	4
54	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

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55	The quantum chemical calculation of NMR two-bond spinâ€“spin coupling constants in the Nâˆ’Â·Â·Â·Hâ€“OHÂ†’ÂNâ€“HÂ·Â·Â·OHâˆ’ switching. Structural Chemistry, 2012, 23, 825-830.	2.0	1
56	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
57	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
58	Conformational and tautomeric preferences in 3â€aminoacrylaldehyde: A theoretical study. International Journal of Quantum Chemistry, 2011, 111, 586-595.	2.0	4
59	Influence of substitution on the strength and nature of CHÂ·Â·Â·N hydrogen bond in XCCHÂ·Â·Â·NH‹sub›3‹/sub›complexes. International Journal of Quantum Chemistry, 2011, 111, 961-969.	2.0	15
60	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
61	H-bonded complexes of uracil with parent nitrosamine: A quantum chemical study. Computational and Theoretical Chemistry, 2011, 965, 211-220.	2.5	82
62	Molecular interactions in methylimidazolium tetrafluoroborate ionic liquid ([Mim+][BF4âˆ’]): 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
63	Influence of HOClâ€¦O‹sub›3‹/sub›and HOClâ€¦HOCl interactions on the stability of O‹sub›3‹/sub›(HOCl)‹sub›2‹/sub›complexes: a theoretical study. Molecular Simulation, 2011, 37, 386-393.	2.0	0
64	Interaction between NH‹sub›2‹/sub›NO and H‹sub›2‹/sub›O‹sub›2‹/sub›: A quantum chemistry study. International Journal of Quantum Chemistry, 2010, 110, 1972-1981.	2.0	4
65	Adsorption of parent nitrosamine on the nanocrystaline Hâ€“zeolite: A theoretical study. Applied Surface Science, 2010, 256, 7575-7582.	6.1	10
66	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
67	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
68	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
69	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
70	Quantum chemical study of the O3â€“HONO complex. Chemical Physics Letters, 2009, 476, 168-173.	2.6	6
71	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
72	DFT study of the biphenyleneâ€“NO complexes formed in nitration mechanism. Journal of Physical Organic Chemistry, 2008, 21, 971-978.	1.9	10

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73	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
74	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
75	Interaction between O3 and H2O2: A theoretical study. Chemical Physics Letters, 2008, 460, 72-78.	2.6	12
76	Atomic and electronic structures of finite single-walled BN nanotubes: Hybrid DFT calculations. Computational and Theoretical Chemistry, 2008, 856, 46-58.	1.5	10
77	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
78	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
79	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
80	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
81	Generalized Anomeric Effect in CH4â^'nClnS. Energetic and NBO Analyses. Bulletin of the Chemical Society of Japan, 2007, 80, 1323-1330.	3.2	3
82	Blue-shifted H-bond in aromatic sulfines: An ab initio calculation. International Journal of Quantum Chemistry, 2007, 107, 1559-1565.	2.0	2
83	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
84	NBO and AIM analyses of the anomeric effect in fluoromethanthiol. Computational and Theoretical Chemistry, 2006, 772, 65-73.	1.5	12
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	Anomeric effect and rotational barrier in fluoromethanol: A theoretical study. Computational and Theoretical Chemistry, 2005, 726, 141-148.	1.5	30
87	AIM and NBO analyses of Nâ€“N rotational barrier in monocyclic nitrosamine compounds. Chemical Physics Letters, 2005, 409, 212-218.	2.6	15
88	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
89	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
90	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