Reza Omidyan

List of Publications by Year
in descending order

42 papers	456 citations	840585 11 h-index	794469 19 g-index
42 all docs	42 docs citations	42 times ranked	417 citing authors

#	Article	IF	Citations
1	Theoretical comparative survey on the structure and electronic properties of first row transition metal substituted Keggin type polyoxometalates. Journal of Solid State Chemistry, 2022, 305, 122667.	1.4	4
2	Insights into the effect of distal histidine and water hydrogen bonding on NO ligation to ferrous and ferric heme: a DFT study. RSC Advances, 2022, 12, 4703-4713.	1.7	0
3	Excited state deactivation mechanisms of protonated adenine: a theoretical study. Physical Chemistry Chemical Physics, 2022, 24, 14898-14908.	1.3	1
4	Theoretical insights on the excited-state-deactivation mechanisms of protonated thymine and cytosine. Physical Chemistry Chemical Physics, 2021, 23, 8916-8925.	1.3	3
5	Molecular dynamics simulation study of curcumin interaction with nano-micelle of PNIPAAm-b-PEG co-polymer as a smart efficient drug delivery system. Journal of Molecular Liquids, 2021, 332, 115862.	2.3	30
6	Theoretical insights on the effect of environments on binding of CO to the Heme :Ferrous and Ferric systems. Journal of Molecular Liquids, 2021, 344, 117961.	2.3	1
7	DFT study of Î±-Keggin, lacunary Keggin, and iron^{IIâ€“VI} substituted Keggin polyoxometalates: the effect of oxidation state and axial ligand on geometry, electronic structures and oxygen transfer. RSC Advances, 2020, 10, 33718-33730.	1.7	5
8	Excited State Deactivation Mechanism in Protonated Uracil: New Insights from Theoretical Studies. Journal of Physical Chemistry A, 2020, 124, 5089-5097.	1.1	7
9	Water binding to FeIIIhemes studied in a cooled ion trap: characterization of a strong â€˜weakâ€™ ligand. Physical Chemistry Chemical Physics, 2019, 21, 21329-21340.	1.3	10
10	Theoretical insights on nonradiative deactivation mechanisms of protonated xanthine. Journal of Photochemistry and Photobiology A: Chemistry, 2019, 385, 112067.	2.0	7
11	The dramatic effect of N-methylimidazole on trans axial ligand binding to ferric heme: experiment and theory. Physical Chemistry Chemical Physics, 2019, 21, 1750-1760.	1.3	11
12	Photophysical and optoelectronic properties of a platinum(II) complex and its derivatives, designed as a highly efficient OLED emitter: A theoretical study. International Journal of Quantum Chemistry, 2019, 119, e25793.	1.0	8
13	Photochromism of 2-(2-Hydroxyphenyl) Benzothiazole (HBT) and Its Derivatives: A Theoretical Study. Journal of Physical Chemistry A, 2018, 122, 3182-3189.	1.1	13
14	Excited-State Proton Transfer in Thiazolo-[4, 5-d]thiazo Heterocyclic Systems and the Geometry Alterationsâ€™ Effect on Photophysical Characters: A Theoretical Study. Journal of Physical Chemistry A, 2018, 122, 2653-2662.	1.1	7
15	Photophysics of Protonated and Microhydrated 2-Aminobenzaldehyde: Theoretical Insights into Photoswitchability of Protonated Systems. Journal of Physical Chemistry A, 2018, 122, 8849-8857.	1.1	4
16	Optical properties of Î²-brominated meso-tetraphenylporphyrins: Comparative experimental and computational studies. Journal of Porphyrins and Phthalocyanines, 2018, 22, 646-657.	0.4	9
17	Solvation effect on isomer stability and electronic structures of protonated serotonin. Chemical Physics Letters, 2017, 679, 90-96.	1.2	1
18	Protonated serotonin: Geometry, electronic structures and photophysical properties. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 182, 8-16.	2.0	2

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19	Excited-state intramolecular proton transfer and photoswitching in hydroxyphenyl-imidazopyridine derivatives: A theoretical study. Journal of Chemical Physics, 2016, 145, 184303.	1.2	11
20	Electronically excited state of neutral/protonated, indole/5-hydroxyinodoleâ€“water clusters: a theoretical study. RSC Advances, 2016, 6, 33148-33158.	1.7	12
21	The influence of protonation on the structure and spectral properties of porphine: UV-vis, ¹H NMR and ab initio studies. RSC Advances, 2016, 6, 82219-82226.	1.7	10
22	Excited State Proton Transfer and Deactivation Mechanism of 2-(4â€²-Amino-2â€²-hydroxyphenyl)-1H-imidazo-[4,5-c]pyridine and Its Analogues: A Theoretical Study. Journal of Physical Chemistry A, 2016, 120, 1012-1019.	1.1	16
23	Electronically Excited States of Neutral, Protonated Î±-Naphthol and Their Water Clusters: A Theoretical Study. Journal of Physical Chemistry A, 2015, 119, 6650-6660.	1.1	5
24	Excited-state deactivation mechanisms of protonated and neutral phenylalanine: a theoretical study. RSC Advances, 2015, 5, 29032-29039.	1.7	1
25	A theoretical exploration on electronically excited states of protonated furan and thiophene. Photochemical and Photobiological Sciences, 2015, 14, 2261-2269.	1.6	2
26	A theoretical exploration of the nonradiative deactivation of hydrogen-bond complexes: isoindoleâ€“pyridine and quinolineâ€“pyrrole. RSC Advances, 2015, 5, 97619-97628.	1.7	3
27	Photophysics and photochemistry of cis- and trans-hydroquinone, catechol and their ammonia clusters: a theoretical study. Photochemical and Photobiological Sciences, 2015, 14, 457-464.	1.6	6
28	Electronic and vibrational spectra of protonated benzaldehyde-water clusters, [BZ-(H2O)nâ‰¥5]H+: Evidence for ground-state proton transfer to solvent for n â‰¥ 3. Journal of Chemical Physics, 2014, 140, 124314.	1.2	26
29	Protonation effect on the electronic properties of 2-pyridone monomer, dimer and its water clusters: A theoretical study. Journal of Chemical Physics, 2014, 140, 024315.	1.2	10
30	Photophysics of a Schiff base: theoretical exploration of the excited-state deactivation mechanisms of N-salicilydenemethylfurylamine (SMFA). Physical Chemistry Chemical Physics, 2014, 16, 2417-2424.	1.3	9
31	Excited state deactivation pathways of neutral/protonated anisole and p-fluoroanisole: a theoretical study. Physical Chemistry Chemical Physics, 2014, 16, 11679-11689.	1.3	9
32	Hydrogen bond strengthening of cisâ€“trans glyoxal dimers in electronic excited states: A theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 122, 337-342.	2.0	5
33	Electronically excited states of protonated phenol and para-substituted phenol. Chemical Physics Letters, 2013, 555, 19-25.	1.2	8
34	Microhydration Effects on the Electronic Properties of Protonated Phenol: A Theoretical Study. Journal of Physical Chemistry A, 2013, 117, 12842-12850.	1.1	6
35	Theoretical Investigation of Excited State Proton Transfer Process in the N-Salicylidene-2-bromoethylamine. Journal of Physical Chemistry A, 2013, 117, 718-725.	1.1	15
36	Porphine core saddling: Effects on the HOMO/LUMO gap and the macrocycle bond lengths and bond angles. Polyhedron, 2013, 49, 36-40.	1.0	8

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37	Electronically Excited States of Protonated Aromatic Hydrocarbons: Phenanthrene and Pyrene. Journal of Physical Chemistry A, 2013, 117, 2499-2507.	1.1	12
38	Protonated salicylaldehyde: Electronic properties. Chemical Physics, 2012, 399, 224-231.	0.9	19
39	Substitution effects on the UVâ€“vis and 1H NMR spectra of the dications of meso and/or Î² substituted porphyrins with trifluoroacetic acid: Electron-deficient porphyrins compared to the electron-rich ones. Inorganic Chemistry Communication, 2011, 14, 1827-1832.	1.8	32
40	Protonation effect on the electronic structure of small PAHs: Acenaphthylene and Acenaphthene. Chemical Physics Letters, 2011, 518, 15-20.	1.2	4
41	Effect of protonation on the electronic structure of aromatic molecules: naphthaleneH+. Physical Chemistry Chemical Physics, 2010, 12, 14456.	1.3	66
42	Protonated Benzene Dimer: An Experimental and Ab Initio Study. Journal of the American Chemical Society, 2009, 131, 11091-11097.	6.6	38