Palanisamy Deepa

List of Publications by Year
in descending order

30	366	759233 12	794594 19
papers	citations	h-index	g-index

30	30	30	323
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Halogen bonds in crystal TTF derivatives: an ab initio quantum mechanical study. Physical Chemistry Chemical Physics, 2014, 16, 2038-2047.	2.8	46
2	On the origin of the substantial stabilisation of the electron-donor 1,3-dithiole-2-thione-4-carboxyclic acidâ‹¯I‹sub›2‹/sub›and DABCOâ‹¯I‹sub›2‹/sub›complexes. Physical Chemistry Chemical Physics, 2014, 16, 6679-6686.	2.8	31
3	Interactions of anticancer drugs with usual and mismatch base pairs â€" Density functional theory studies. Biophysical Chemistry, 2008, 136, 50-58.	2.8	26
4	Do resonance-assisted intramolecular halogen bonds exist without a charge transfer and a Ïƒ-hole?. Physical Chemistry Chemical Physics, 2015, 17, 27496-27508.	2.8	26
5	Theoretical investigation of interaction between psoralen and altretamine with stacked DNA base pairs. Materials Science and Engineering C, 2012, 32, 423-431.	7.3	25
6	Why Is the L-Shaped Structure of X‹sub›2‹/sub›Â·Â·Â·X‹sub›2‹/sub› (X = F, Cl, Br, I) Complexes More Stable Than Other Structures?. Journal of Physical Chemistry A, 2014, 118, 3846-3855.	2.5	21
7	Studies on the Ïƒâ€“hole bonds (halogen, chalcogen, pnicogen and carbon bonds) based on the orientation of crystal structure. Molecular Physics, 2016, 114, 3629-3642.	1.7	20
8	Characteristics of a Ïƒ-Hole and the Nature of a Halogen Bond. Topics in Current Chemistry, 2014, 359, 1-25.	4.0	19
9	On the nature of non-covalent interactions in isomers of 2,5-dichloro-1,4-benzoquinone dimers â€“ ground- and excited-state properties. Physical Chemistry Chemical Physics, 2014, 16, 19928-19940.	2.8	16
10	Studies on Tautomeric Forms of Guanine-Cytosine Base Pairs of Nucleic Acids and Their Interactions with Water Molecules. Journal of Biomolecular Structure and Dynamics, 2008, 25, 733-746.	3.5	15
11	A theoretical perspective of the nature of hydrogen-bond types â€“ the atoms in molecules approach. Molecular Physics, 2014, 112, 1609-1623.	1.7	15
12	The nature of hydrogen bonding in‹i›R‹/i›‹sup›2‹/sup›‹sub›2‹/sub›(8) crystal motifs â€“ a computational exploration. Molecular Physics, 2014, 112, 3195-3205.	1.7	14
13	Structural properties and the effect of platinum drugs with DNA base pairs. Structural Chemistry, 2013, 24, 583-595.	2.0	13
14	Hydrogen-bonding studies of amino acid side-chains with DNA base pairs. Molecular Physics, 2011, 109, 1995-2008.	1.7	10
15	Structural properties and the effect of 2,6â€diaminoanthraquinone on Gâ€tetrad, nonâ€Câ€tetrads, and mixed tetradsâ€"A density functional theory study. International Journal of Quantum Chemistry, 2011, 111, 3239-3250.	2.0	8
16	First and second coordination spheres in 8-azaxanthinato salts of divalent metal aquacomplexes â€“ Ab initio and DFT study. Polyhedron, 2011, 30, 1431-1445.	2.2	8
17	An Overview of the Factors Influencing CK2 Ligands and the Impact of Crystal Waters: A Theoretical Study. Crystal Growth and Design, 2017, 17, 1299-1315.	3.0	8
18	Understanding the potency of fatty acids with the amino acid side chains of bovine Î² lactoglobulinâ€"A quantum chemical approach. Journal of Molecular Graphics and Modelling, 2017, 74, 105-116.	2.4	7

#	Article	IF	Citations
19	Does the occurrence of resonance (by the delocalization of radical/cationic/anionic charges) induce the existence of intramolecular halogenâ€“halogen contacts?. RSC Advances, 2016, 6, 66870-66878.	3.6	6
20	Does the presence of water clusters induce the binding affinity of CK2 halogen ligands?: A quantum chemical perspective study. International Journal of Quantum Chemistry, 2018, 118, e25644.	2.0	6
21	Hybrid DFT study on non-covalent interactions and their influence on pKa's of magnesium-carboxylate complexes. Journal of Molecular Graphics and Modelling, 2018, 85, 13-24.	2.4	5
22	A quantum chemical perspective on the potency of electron donors and acceptors in pnicogen bonds (AS...N, P...N, N...N). Journal of Molecular Modeling, 2020, 26, 11.	1.8	5
23	Understanding the potency of malarial ligand (D44) in plasmodium FKBP35 and modelled halogen atom (Br, Cl, F) functional groups. Journal of Molecular Graphics and Modelling, 2020, 97, 107553.	2.4	5
24	Topological analysis of metalâ€“ligand and hydrogen bonds in transition metal hybrid structures â€“ A computational study. Polyhedron, 2016, 115, 193-203.	2.2	4
25	An overview about the impact of hinge region towards the anticancer binding affinity of the Ck2 ligands: a quantum chemical analysis. Journal of Biomolecular Structure and Dynamics, 2019, 37, 3859-3876.	3.5	3
26	Synthesis and Experimental Studies on Supramolecular Synthons of Aminoguanidinium Carboxylates: A Case Study of I€â€HoleBonded Carbon Bonding via Theoretical Approaches. ChemistrySelect, 2018, 3, 10032-10048.	1.5	1
27	Does the stability of the stacking motif surpass the planar motif in 2-amino-4-nitrophenol? â€” a CCSD(T) analysis. Journal of Molecular Modeling, 2019, 25, 6.	1.8	1
28	Rising trend on the halogen and non-halogen derivatives (Br, Cl, CF₃, F, CH₃) Tj ETQq0 0 0 rgBT /Overlock 10 T Biomolecular Structure and Dynamics, 2022, 40, 449-467.	3.5	1
29	Understanding the impact of anticancer halogenated inhibitors and various functional groups (Xâ€‰=â€‰Cl,) Tj ETQq1 1 0.784314 rg Biomolecular Structure and Dynamics, 2022, 40, 5036-5052.	3.5	1
30	Understanding the nature of Metal Oxalato Complexes with Purine Nucleobase- A Quantum Chemical approach. International Journal of Molecular and Theoretical Physics, 2017, 1, 1-10.	0.3	0