Jurgens H De Lange

List of Publications by Year
in descending order

16	266	1040056 9	996975 15
papers	citations	h-index	g-index

17	17	17	297
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Physical Nature of Interactions in Zn^{II} Complexes with 2,2â€²-Bipyridyl: Quantum Theory of Atoms in Molecules (QTAIM), Interacting Quantum Atoms (IQA), Noncovalent Interactions (NCI), and Extended Transition State Coupled with Natural Orbitals for Chemical Valence (ETS-NOCV) Comparative Studies. Journal of Physical Chemistry A, 2014, 118, 623-637.	2.5	81
2	Evaluating common QTAIM and NCI interpretations of the electron density concentration through IQA interaction energies and 1D cross-sections of the electron and deformation density distributions. Computational and Theoretical Chemistry, 2015, 1053, 60-76.	2.5	50
3	Adsorption of antiretroviral drugs, efavirenz and nevirapine from aqueous solution by graphene wool: Kinetic, equilibrium, thermodynamic and computational studies. Applied Surface Science Advances, 2021, 6, 100157.	6.8	30
4	Synthesis, structure and DFT study of asymmetrical NHC complexes of cymantrene derivatives and their application in the dehydrogenative dimerization reaction of thiols. Journal of Organometallic Chemistry, 2017, 840, 11-22.	1.8	16
5	Origin of Hydrocarbons Stability from a Computational Perspective: A Case Study of Orthoâ€Xylene Isomers. ChemPhysChem, 2020, 21, 494-502.	2.1	15
6	Exploring fundamental differences between red- and blue-shifted intramolecular hydrogen bonds using FAMSEC, FALDI, IQA and QTAIM. Structural Chemistry, 2017, 28, 1429-1444.	2.0	13
7	Toward deformation densities for intramolecular interactions without radical reference states using the fragment, atom, localized, delocalized, and interatomic (FALDI) charge density decomposition scheme. Journal of Computational Chemistry, 2017, 38, 981-997.	3.3	12
8	FALDIâ€based decomposition of an atomic interaction line leads to 3D representation of the multicenter nature of interactions. Journal of Computational Chemistry, 2018, 39, 973-985.	3.3	10
9	Quantifying individual (anti)bonding molecular orbitalsâ€™ contributions to chemical bonding. Physical Chemistry Chemical Physics, 2019, 21, 20988-20998.	2.8	10
10	FALDIâ€based criterion for and the origin of an electron density bridge with an associated (3,â€“1) critical point on Bader's molecular graph. Journal of Computational Chemistry, 2018, 39, 2283-2299.	3.3	8
11	Exact and exclusive electron localization indices within QTAIM atomic basins. Journal of Computational Chemistry, 2018, 39, 1517-1530.	3.3	7
12	The CHÂ·Â·Â·HC interaction in biphenyl is a delocalized, molecularâ€wide and entirely nonâ€classical interaction: Results from FALDI analysis. Journal of Computational Chemistry, 2021, 42, 706-718.	3.3	7
13	Gold(I) Hydrides as Proton Acceptors in Dihydrogen Bond Formation. ChemPhysChem, 2017, 18, 2288-2294.	2.1	3
14	Molecular Orbitals Support Energy-Stabilizing â€œBondingâ€•Nature of Baderâ€™s Bond Paths. Journal of Physical Chemistry A, 2020, 124, 5523-5533.	2.5	2
15	Comparison of DAFH and FALDI-like approaches. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	1
16	Characterization of bonding modes in metal complexes through electron density crossâ€sections. Journal of Computational Chemistry, 2020, 41, 2695-2706.	3.3	1