# Jurgens H De Lange

List of Publications by Year
in descending order



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|---|---|---|---|
| 16 papers | 266 citations | 1040018 9 h-index | 996954 15 g-index |
| 17 all docs | 17 docs citations | 17 times ranked | 297 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Physical Nature of Interactions in Zn<sup>II</sup> 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 |