Arnout Ceulemans

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3011967/publications.pdf

Version: 2024-02-01

46	1,117	394421	395702
papers	citations	19 h-index	33 g-index

46	46	46	1147
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Room-temperature magnetic anisotropy of lanthanide complexes: A model study for various coordination polyhedra. Journal of Chemical Physics, 2002, 116, 4673-4685.	3.0	98
2	Disk Aromaticity of the Planar and Fluxional Anionic Boron Clusters B₂₀^{â˜’/2â˜’}. Chemistry - A European Journal, 2012, 18, 4510-4512.	3.3	90
3	Substituent-Induced Circular Dichroism in Phthalocyanines. Journal of the American Chemical Society, 1999, 121, 12018-12028.	13.7	84
4	The structure of Jahnâ€“Teller surfaces. Journal of Chemical Physics, 1987, 87, 5374-5385.	3.0	75
5	The boron buckyball has an unexpected Th symmetry. Chemical Physics Letters, 2008, 450, 175-177.	2.6	75
6	Chemical bonding in the boron buckyball. Chemical Physics Letters, 2008, 461, 226-228.	2.6	53
7	Singletâ˜’Triplet Energy Gaps of Gas-Phase RNA and DNA Bases. A Quantum Chemical Study. Journal of Physical Chemistry A, 2004, 108, 6554-6561.	2.5	52
8	Improved Replica Exchange Method for Native-State Protein Sampling. Journal of Chemical Theory and Computation, 2011, 7, 231-237.	5.3	48
9	Helical Structure of Xylose-DNA. Journal of the American Chemical Society, 2010, 132, 587-595.	13.7	47
10	The leapfrog principle for boron fullerenes: a theoretical study of structure and stability of B112. Physical Chemistry Chemical Physics, 2011, 13, 7524.	2.8	44
11	Particle on a Boron Disk: Ring Currents and Disk Aromaticity in B₂₀^{2â€“}. Inorganic Chemistry, 2013, 52, 10595-10600.	4.0	44
12	Quantum rules for planar boron nanoclusters. Physical Chemistry Chemical Physics, 2014, 16, 18311-18318.	2.8	33
13	Theoretical Study on the Regioselectivity of the B₈₀ Buckyball in Electrophilic and Nucleophilic Reactions Using DFT-Based Reactivity Indices. Journal of Physical Chemistry A, 2011, 115, 9069-9080.	2.5	32
14	The construction of symmetric orbitals for molecular clusters. Molecular Physics, 1985, 54, 161-181.	1.7	26
15	Molecular dynamics study of dipalmitoylphosphatidylcholine lipid layer self-assembly onto a single-walled carbon nanotube. Nano Research, 2009, 2, 945-954.	10.4	25
16	Xylonucleic acid: synthesis, structure, and orthogonal pairing properties. Nucleic Acids Research, 2015, 43, 7189-7200.	14.5	23
17	Solution Structure and Conformational Dynamics of Deoxyxylonucleic Acids (dXNA): An Orthogonal Nucleic Acid Candidate. Chemistry - A European Journal, 2012, 18, 869-879.	3.3	21
18	Absorption and Fluorescence of 3-Methylindole:â€‰ A Theoretical Study, Including H2O Interactions. Journal of Physical Chemistry A, 2004, 108, 7577-7583.	2.5	19

#	Article	IF	Citations
19	Jahnâ€“Teller instability in cationic boron and carbon buckyballs B80+ and C60+: a comparative study. Physical Chemistry Chemical Physics, 2013, 15, 2829.	2.8	19
20	Ab Initio Calculations of the Trigonal and Zero-Field Splittings in Trischelated Diketonato Complexes of Trivalent Chromium. Inorganic Chemistry, 1998, 37, 5227-5232.	4.0	17
21	Formation of the quasi-planar B₅₀ boron cluster: topological path from B₁₀ and disk aromaticity. Physical Chemistry Chemical Physics, 2019, 21, 7039-7044.	2.8	17
22	Theoretical Study of Alkali Metal Pyrrolides in Comparison with nHâ^'Pyrrole. Journal of Physical Chemistry A, 2003, 107, 5427-5438.	2.5	15
23	Molecular Dynamic Indicators of the Photoswitching Properties of Green Fluorescent Proteins. Journal of Physical Chemistry B, 2015, 119, 12007-12016.	2.6	13
24	Is C50 a superaromat? Evidence from electronic structure and ring current calculations. Physical Chemistry Chemical Physics, 2016, 18, 11653-11660.	2.8	12
25	Hiatus in the spherical shell model of fullerenes. Physical Chemistry Chemical Physics, 2004, 6, 238-241.	2.8	11
26	Conductance of a copper-nanotube bundle interface: Impact of interface geometry and wave-function interference. Physical Review B, 2008, 77, .	3.2	10
27	Jahnâ€“Teller Instability of Icosahedral [W@Au12]â^. Journal of Chemical Theory and Computation, 2014, 10, 613-622.	5.3	10
28	Systematic Excited State Studies of Reversibly Switchable Fluorescent Proteins. Journal of Chemical Theory and Computation, 2018, 14, 3163-3172.	5.3	10
29	Exchange interactions in Ti₂Cl³⁻₉and the magnetic susceptibility tensor. Molecular Physics, 1999, 97, 1197-1202.	1.7	9
30	Thermal Isomerization Mechanism in Dronpa and Its Mutants. Journal of Physical Chemistry B, 2016, 120, 12820-12825.	2.6	9
31	Molecular Dynamics of Double Stranded Xylo-Nucleic Acid. Journal of Chemical Theory and Computation, 2017, 13, 5028-5038.	5.3	9
32	The butterfly geometry: A Jahnâ€“Teller view. Journal of Chemical Physics, 1986, 84, 6442-6451.	3.0	8
33	The Polyhedral State of Molecular Matter. European Journal of Inorganic Chemistry, 2002, 2002, 1571-1581.	2.0	8
34	Valence bonds in elongated boron clusters. International Journal of Quantum Chemistry, 2018, 118, e25575.	2.0	8
35	Jahn and Tellers Last Case: The Icosahedral Sextet, Î“9Ã—(g+2h). ChemPhysChem, 2007, 8, 64-67.	2.1	7
36	The quantization of the Rabi Hamiltonian. Journal of Physics A: Mathematical and Theoretical, 2017, 50, 114002.	2.1	6

#	Article	IF	Citations
37	Jahnâ€“Teller Distortion in Polyoligomeric Silsesquioxane (POSS) Cations. Journal of Physical Chemistry A, 2015, 119, 4237-4243.	2.5	5
38	Valence bonds in planar and quasi-planar boron disks. Physical Chemistry Chemical Physics, 2019, 21, 729-735.	2.8	5
39	On the Possibility of a Pseudo Atomic Ground State for CrF2:â€‰Ab-Initio and Crystal Field Calculations Including Spinâ^'Orbit Coupling. Journal of Physical Chemistry A, 1997, 101, 5813-5817.	2.5	4
40	Structure, stability and bonding of the leapfrog B 24 0 ,Â±1,Â±2. Journal of Computational Chemistry, 2021, 42, 72-80.	3.3	4
41	Construction of the Î“9Ã— (g+ 2h) Jahnâ€“Teller Hamiltonian. Molecular Physics, 2006, 104, 3173-3185.	1.7	3
42	The Quantization of the E âŠ— e Jahnâ€“Teller Hamiltonian. Journal of Physical Chemistry A, 2017, 121, 7246-7254.	2.5	3
43	A comparison of the chemical bonding and reactivity of Si8H8O12 and Ge8H8O12: A theoretical study. Journal of Chemical Physics, 2021, 154, 164305.	3.0	2
44	Ansatz for the Jahnâ€“Teller triplet instability. Journal of Chemical Physics, 2020, 153, 174110.	3.0	2
45	Description of nanotubes using line group symmetry. AIP Conference Proceedings, 2001, , .	0.4	1
46	Directed Graphs and Induced Magnetic Multipoles in Polycyclic Hydrocarbons. Bulletin of the Chemical Society of Japan, 2015, 88, 1553-1560.	3.2	1