

Arnout Ceulemans

List of Publications by Year in descending order

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46
papers

1,117
citations

394421

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times ranked

1147
citing authors

#	ARTICLE	IF	CITATIONS
1	Structure, stability and bonding of the leapfrog B ₂₄ O ₄₂ , $\hat{A}\pm 1, \hat{A}\pm 2$. Journal of Computational Chemistry, 2021, 42, 72-80.	3.3	4
2	A comparison of the chemical bonding and reactivity of Si ₈ H ₈ O ₁₂ and Ge ₈ H ₈ O ₁₂ : A theoretical study. Journal of Chemical Physics, 2021, 154, 164305.	3.0	2
3	Ansatz for the Jahn–Teller triplet instability. Journal of Chemical Physics, 2020, 153, 174110.	3.0	2
4	Valence bonds in planar and quasi-planar boron disks. Physical Chemistry Chemical Physics, 2019, 21, 729-735.	2.8	5
5	Formation of the quasi-planar B ₅₀ boron cluster: topological path from B ₁₀ and disk aromaticity. Physical Chemistry Chemical Physics, 2019, 21, 7039-7044.	2.8	17
6	Valence bonds in elongated boron clusters. International Journal of Quantum Chemistry, 2018, 118, e25575.	2.0	8
7	Systematic Excited State Studies of Reversibly Switchable Fluorescent Proteins. Journal of Chemical Theory and Computation, 2018, 14, 3163-3172.	5.3	10
8	The quantization of the Rabi Hamiltonian. Journal of Physics A: Mathematical and Theoretical, 2017, 50, 114002.	2.1	6
9	The Quantization of the $\langle i \rangle E \langle /i \rangle$ – $\langle i \rangle e \langle /i \rangle$ Jahn–Teller Hamiltonian. Journal of Physical Chemistry A, 2017, 121, 7246-7254.	2.5	3
10	Molecular Dynamics of Double Stranded Xylo-Nucleic Acid. Journal of Chemical Theory and Computation, 2017, 13, 5028-5038.	5.3	9
11	Thermal Isomerization Mechanism in Dronpa and Its Mutants. Journal of Physical Chemistry B, 2016, 120, 12820-12825.	2.6	9
12	Is C ₅₀ a superaromat? Evidence from electronic structure and ring current calculations. Physical Chemistry Chemical Physics, 2016, 18, 11653-11660.	2.8	12
13	Directed Graphs and Induced Magnetic Multipoles in Polycyclic Hydrocarbons. Bulletin of the Chemical Society of Japan, 2015, 88, 1553-1560.	3.2	1
14	Jahn–Teller Distortion in Polyoligomeric Silsesquioxane (POSS) Cations. Journal of Physical Chemistry A, 2015, 119, 4237-4243.	2.5	5
15	Molecular Dynamic Indicators of the Photoswitching Properties of Green Fluorescent Proteins. Journal of Physical Chemistry B, 2015, 119, 12007-12016.	2.6	13
16	Xylonucleic acid: synthesis, structure, and orthogonal pairing properties. Nucleic Acids Research, 2015, 43, 7189-7200.	14.5	23
17	Quantum rules for planar boron nanoclusters. Physical Chemistry Chemical Physics, 2014, 16, 18311-18318.	2.8	33
18	Jahn–Teller Instability of Icosahedral [W@Au ₁₂] ⁺ . Journal of Chemical Theory and Computation, 2014, 10, 613-622.	5.3	10

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19	Jahn–Teller instability in cationic boron and carbon buckyballs B ₈₀ ⁺ and C ₆₀ ⁺ : a comparative study. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 2829.	2.8	19
20	Particle on a Boron Disk: Ring Currents and Disk Aromaticity in B ₂₀ ²⁺ . <i>Inorganic Chemistry</i> , 2013, 52, 10595-10600.	4.0	44
21	Disk Aromaticity of the Planar and Fluxional Anionic Boron Clusters B ₂₀ ⁻² . <i>Chemistry - A European Journal</i> , 2012, 18, 4510-4512.	3.3	90
22	Solution Structure and Conformational Dynamics of Deoxyxylonucleic Acids (dXNA): An Orthogonal Nucleic Acid Candidate. <i>Chemistry - A European Journal</i> , 2012, 18, 869-879.	3.3	21
23	The leapfrog principle for boron fullerenes: a theoretical study of structure and stability of B ₁₁₂ . <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 7524.	2.8	44
24	Theoretical Study on the Regioselectivity of the B ₈₀ Buckyball in Electrophilic and Nucleophilic Reactions Using DFT-Based Reactivity Indices. <i>Journal of Physical Chemistry A</i> , 2011, 115, 9069-9080.	2.5	32
25	Improved Replica Exchange Method for Native-State Protein Sampling. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 231-237.	5.3	48
26	Helical Structure of Xylose-DNA. <i>Journal of the American Chemical Society</i> , 2010, 132, 587-595.	13.7	47
27	Molecular dynamics study of dipalmitoylphosphatidylcholine lipid layer self-assembly onto a single-walled carbon nanotube. <i>Nano Research</i> , 2009, 2, 945-954.	10.4	25
28	The boron buckyball has an unexpected Th symmetry. <i>Chemical Physics Letters</i> , 2008, 450, 175-177.	2.6	75
29	Chemical bonding in the boron buckyball. <i>Chemical Physics Letters</i> , 2008, 461, 226-228.	2.6	53
30	Conductance of a copper-nanotube bundle interface: Impact of interface geometry and wave-function interference. <i>Physical Review B</i> , 2008, 77, .	3.2	10
31	Jahn and Tellers Last Case: The Icosahedral Sextet, $\hat{I}^{9A_1-(g+2h)}$. <i>ChemPhysChem</i> , 2007, 8, 64-67.	2.1	7
32	Construction of the $\hat{I}^{9A_1-(g+2h)}$ Jahn–Teller Hamiltonian. <i>Molecular Physics</i> , 2006, 104, 3173-3185.	1.7	3
33	Hiatus in the spherical shell model of fullerenes. <i>Physical Chemistry Chemical Physics</i> , 2004, 6, 238-241.	2.8	11
34	Absorption and Fluorescence of 3-Methylindole: A Theoretical Study, Including H ₂ O Interactions. <i>Journal of Physical Chemistry A</i> , 2004, 108, 7577-7583.	2.5	19
35	Singlet–Triplet Energy Gaps of Gas-Phase RNA and DNA Bases. A Quantum Chemical Study. <i>Journal of Physical Chemistry A</i> , 2004, 108, 6554-6561.	2.5	52
36	Theoretical Study of Alkali Metal Pyrrolides in Comparison with nH–Pyrrole. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5427-5438.	2.5	15

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37	The Polyhedral State of Molecular Matter. European Journal of Inorganic Chemistry, 2002, 2002, 1571-1581.	2.0	8
38	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
39	Description of nanotubes using line group symmetry. AIP Conference Proceedings, 2001, , .	0.4	1
40	Exchange interactions in Ti_2Cl_3 and the magnetic susceptibility tensor. Molecular Physics, 1999, 97, 1197-1202.	1.7	9
41	Substituent-Induced Circular Dichroism in Phthalocyanines. Journal of the American Chemical Society, 1999, 121, 12018-12028.	13.7	84
42	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
43	On the Possibility of a Pseudo Atomic Ground State for CrF_2 : Ab-Initio and Crystal Field Calculations Including Spin-Orbit Coupling. Journal of Physical Chemistry A, 1997, 101, 5813-5817.	2.5	4
44	The structure of Jahn-Teller surfaces. Journal of Chemical Physics, 1987, 87, 5374-5385.	3.0	75
45	The butterfly geometry: A Jahn-Teller view. Journal of Chemical Physics, 1986, 84, 6442-6451.	3.0	8
46	The construction of symmetric orbitals for molecular clusters. Molecular Physics, 1985, 54, 161-181.	1.7	26