Denis Hagebaum-Reignier

List of Publications by Year
in descending order

32	380	840776 11	794594 19
papers	citations	h-index	g-index

32	32	32	521
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Stereoselective Syntheses, Structures, and Properties of Extremely Distorted Chiral Nanographenes Embedding Hextuple Helicenes. Angewandte Chemie - International Edition, 2020, 59, 3264-3271.	13.8	67
2	Formation mechanism of glycolaldehyde and ethylene glycol in astrophysical ices from HCO^{â€¢}and^{â€¢}CH₂OH recombination: an experimental study. Monthly Notices of the Royal Astronomical Society, 2015, 453, 1587-1596.	4.4	63
3	HÃ¼ckel-Lewis Projection Method: A â€œWeights Watcherâ€•for Mesomeric Structures. Journal of Physical Chemistry A, 2008, 112, 13256-13262.	2.5	36
4	Stereoselective Syntheses, Structures, and Properties of Extremely Distorted Chiral Nanographenes Embedding Hextuple Helicenes. Angewandte Chemie, 2020, 132, 3290-3297.	2.0	29
5	Analysis of the physical contributions to magnetic couplings in broken symmetry density functional theory approach. Journal of Chemical Physics, 2012, 137, 114106.	3.0	28
6	Bonding of Gold with Unsaturated Species. ChemPhysChem, 2012, 13, 2090-2096.	2.1	25
7	Molecular properties and potential energy surfaces of the cyanides of the groups 1 and 11 metal atoms. Journal of Chemical Physics, 2007, 126, 244313.	3.0	22
8	HÃ¼ckel theory for Lewis structures: HÃ¼ckelâ€“Lewis Configuration Interaction (HL-CI). Computational and Theoretical Chemistry, 2007, 817, 99-109.	1.5	18
9	Visualizing electron delocalization in contorted polycyclic aromatic hydrocarbons. Chemical Science, 2021, 12, 13092-13100.	7.4	17
10	Radical-assisted polymerization in interstellar ice analogues: formyl radical and polyoxymethylene. Monthly Notices of the Royal Astronomical Society, 2019, 486, 1953-1963.	4.4	14
11	First-order correction for bond energy applied to polar molecules: Alkali halides, alkali cyanides, LiCH3, and CH3F. Chemical Physics, 2006, 327, 406-414.	1.9	12
12	Magnetic exchange coupling in bis-nitroxides: a theoretical analysis of the solvent effects. Physical Chemistry Chemical Physics, 2012, 14, 5504.	2.8	9
13	Cold collisions of alkali-metal atoms and chromium atoms. Journal of Physics B: Atomic, Molecular and Optical Physics, 2010, 43, 235208.	1.5	5
14	Recasting wave functions into valence bond structures: A simple projection method to describe excited states. Journal of Computational Chemistry, 2016, 37, 771-779.	3.3	5
15	Multidimensional Isotropic Magnetic Shielding Contour Maps for the Visualization of Aromaticity in ortho-Arynes and Their Reactions. Synthesis, 2022, 54, 4997-5002.	2.3	4
16	Experimental and theoretical studies of the quenching of Li(3p,4p) by N2. Journal of Chemical Physics, 2005, 123, 024303.	3.0	3
17	Study on chemical kinetics of HTOâ€¯+â€¯H2â€¯â†’â€¯H2Oâ€¯+â€¯HT for design of tritium breeding blanket. Fusion Engineering and Design, 2018, 136, 438-441.	1.9	3
18	Using Constraint Programming to Generate Benzenoid Structures in Theoretical Chemistry. Lecture Notes in Computer Science, 2020, , 690-706.	1.3	3

#	Article	IF	Citations
19	HuLiS, a program to teach mesomerism and more. Journal of Physics: Conference Series, 2016, 738, 012015.	0.4	2
20	Potential energy surfaces of the electronic states of Li2F and Li2Fâ˜. Journal of Chemical Physics, 2016, 145, 034306.	3.0	2
21	Localized Structures at the HÃ¼ckel Level, a HÃ¼ckel-Derived Valence Bond Method. Challenges and Advances in Computational Chemistry and Physics, 2016, , 337-360.	0.6	2
22	A generalized Brillouin theorem (GBT)-like implementation to optimize Valence Bond wave function for excited states. Computational and Theoretical Chemistry, 2017, 1116, 184-189.	2.5	2
23	Theoretical chemical ionization rate constants of the concurrent reactions of hydronium ions (H₃O⁺) and oxygen ions (O) with selected organic iodides. Journal of Mass Spectrometry, 2019, 54, 422-428.	1.6	2
24	Computing the Local Aromaticity ofÂBenzenoids Thanks to Constraint Programming. Lecture Notes in Computer Science, 2020, , 673-689.	1.3	2
25	Experimental studies of collisions of excited Li(4p) atoms with C2H4, C2H6, C3H8 and theoretical interpretation of the Liâ€“C2H4 system. Chemical Physics, 2009, 355, 157-163.	1.9	1
26	Planar and pyramidal conformers of the alkaliâ€“ethylene complexes. Chemical Physics Letters, 2010, 487, 214-219.	2.6	1
27	Full-Dimensional Ab Initio Potential Energy Surface and Vibrational Energy Levels of Li2H. Molecules, 2019, 24, 26.	3.8	1
28	Electronic densities and valence bond wave functions. Journal of Chemical Physics, 2022, 156, 204310.	3.0	1
29	BenzAI: A Program to Design Benzenoids with Defined Properties Using Constraint Programming. Journal of Chemical Information and Modeling, 2022, 62, 2811-2820.	5.4	1
30	Calculating Hermitian Forms: The Importance of Considering Singular Points. Bulletin of the Korean Chemical Society, 2020, 41, 254-260.	1.9	0
31	How constraint programming can help chemists to generate Benzenoid structures and assess the local Aromaticity of Benzenoids. Constraints, 2022, 27, 192-248.	0.7	0
32	Resonant Ionic, Covalent Bond, and Steric Characteristics Present in 1Î£u+ States of Li2. Molecules, 2022, 27, 3514.	3.8	0