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	Electronic densities and valence bond wave functions. Journal of Chemical Physics, 2022, 156, 204310.	3.0	1
2	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
3	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
4	Resonant Ionic, Covalent Bond, and Steric Characteristics Present in 1Îžu+ States of Li2. Molecules, 2022, 27, 3514.	3.8	0
5	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
6	Visualizing electron delocalization in contorted polycyclic aromatic hydrocarbons. Chemical Science, 2021, 12, 13092-13100.	7.4	17
7	Calculating Hermitian Forms: The Importance of Considering Singular Points. Bulletin of the Korean Chemical Society, 2020, 41, 254-260.	1.9	0
8	Stereoselective Syntheses, Structures, and Properties of Extremely Distorted Chiral Nanographenes Embedding Hextuple Helicenes. Angewandte Chemie - International Edition, 2020, 59, 3264-3271.	13.8	67
9	Stereoselective Syntheses, Structures, and Properties of Extremely Distorted Chiral Nanographenes Embedding Hextuple Helicenes. Angewandte Chemie, 2020, 132, 3290-3297.	2.0	29
10	Using Constraint Programming to Generate Benzenoid Structures in Theoretical Chemistry. Lecture Notes in Computer Science, 2020, , 690-706.	1.3	3
11	Computing the Local Aromaticity ofÂBenzenoids Thanks to Constraint Programming. Lecture Notes in Computer Science, 2020, , 673-689.	1.3	2
12	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
13	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
14	Full-Dimensional Ab Initio Potential Energy Surface and Vibrational Energy Levels of Li2H. Molecules, 2019, 24, 26.	3.8	1
15	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
16	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
17	HuLiS, a program to teach mesomerism and more. Journal of Physics: Conference Series, 2016, 738, 012015.	0.4	2
18	Potential energy surfaces of the electronic states of Li2F and Li2Fâº. Journal of Chemical Physics, 2016, 145, 034306.	3.0	2

#	Article	IF	Citations
19	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
20	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
21	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
22	Magnetic exchange coupling in bis-nitroxides: a theoretical analysis of the solvent effects. Physical Chemistry Chemical Physics, 2012, 14, 5504.	2.8	9
23	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
24	Bonding of Gold with Unsaturated Species. ChemPhysChem, 2012, 13, 2090-2096.	2.1	25
25	Planar and pyramidal conformers of the alkaliâ€“ethylene complexes. Chemical Physics Letters, 2010, 487, 214-219.	2.6	1
26	Cold collisions of alkali-metal atoms and chromium atoms. Journal of Physics B: Atomic, Molecular and Optical Physics, 2010, 43, 235208.	1.5	5
27	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
28	HÃ¼ckel-Lewis Projection Method: A â€œWeights Watcherâ€•for Mesomeric Structures. Journal of Physical Chemistry A, 2008, 112, 13256-13262.	2.5	36
29	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
30	HÃ¼ckel theory for Lewis structures: HÃ¼ckelâ€“Lewis Configuration Interaction (HL-CI). Computational and Theoretical Chemistry, 2007, 817, 99-109.	1.5	18
31	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
32	Experimental and theoretical studies of the quenching of Li(3p,4p) by N2. Journal of Chemical Physics, 2005, 123, 024303.	3.0	3