

John D Goddard

List of Publications by Year in descending order

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34
papers

1,102
citations

361413

20
h-index

395702

33
g-index

34
all docs

34
docs citations

34
times ranked

1058
citing authors

#	ARTICLE	IF	CITATIONS
1	The Spectral-Structural Relationship of a Series of Oxyluciferin Derivatives. <i>ChemPhysChem</i> , 2015, 16, 396-402.	2.1	15
2	Electronic and optical properties of the five most stable C96 isomers. <i>Chemical Physics Letters</i> , 2015, 625, 64-68.	2.6	1
3	Theoretical studies of the structural, electronic, and ¹⁹ F NMR properties of linear and branched perfluorobutanesulfonate. <i>Canadian Journal of Chemistry</i> , 2013, 91, 1272-1280.	1.1	0
4	The formation and decomposition of firefly dioxetanone. <i>Chemical Physics Letters</i> , 2011, 506, 269-275.	2.6	25
5	Effect of Explicit Water Molecules on the Color-Tuning Mechanism of the Firefly. <i>Chinese Journal of Chemistry</i> , 2011, 29, 2301-2307.	4.9	2
6	A relative approach for determining ring strain energies of heterobicyclic alkenes. <i>Tetrahedron</i> , 2009, 65, 4562-4568.	1.9	35
7	Color-Tuning Mechanism in Firefly Luminescence: Theoretical Studies on Fluorescence of Oxyluciferin in Aqueous Solution Using Time Dependent Density Functional Theory. <i>Journal of Physical Chemistry A</i> , 2008, 112, 9796-9800.	2.5	36
8	Predictions of the Geometries and Fluorescence Emission Energies of Oxyluciferins. <i>Journal of Physical Chemistry A</i> , 2007, 111, 4489-4497.	2.5	37
9	Ruthenium-catalyzed [2+2] cycloadditions between substituted alkynes and norbornadiene: a theoretical study. <i>Tetrahedron</i> , 2007, 63, 7659-7666.	1.9	16
10	Remote Substituent Effects in Ruthenium-Catalyzed [2+2] Cycloadditions: An Experimental and Theoretical Study. <i>Journal of Organic Chemistry</i> , 2006, 71, 3793-3803.	3.2	30
11	Predictions of the electronic absorption and emission spectra of luciferin and oxyluciferins including solvation effects. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2005, 81, 163-170.	3.8	25
12	Ring strain energies: substituted rings, norbornanes, norbornenes and norbornadienes. <i>Tetrahedron</i> , 2004, 60, 8103-8112.	1.9	225
13	Ruthenium-Catalyzed [2 + 2] Cycloadditions between 7-Substituted Norbornadienes and Alkynes: An Experimental and Theoretical Study. <i>Journal of Organic Chemistry</i> , 2004, 69, 8467-8474.	3.2	42
14	Assessment of density functional theory for the prediction of the nature of the oxirene stationary point. <i>Computational and Theoretical Chemistry</i> , 2003, 629, 263-270.	1.5	15
15	Theoretical Study of the Amazing Firefly Bioluminescence: The Formation and Structures of the Light Emitters. <i>Journal of the American Chemical Society</i> , 2003, 125, 6962-6971.	13.7	132
16	Practical failures from the inclusion of exact exchange: how much exact exchange is appropriate?. <i>Molecular Physics</i> , 2002, 100, 483-497.	1.7	22
17	Consequences of accidental degeneracy within density functional theory: the enigmatic structure of boron nitrosyl. <i>Chemical Physics Letters</i> , 2002, 356, 7-13.	2.6	2
18	Is density functional theory free of spatial symmetry breaking? The case of the linear carbon radical cations: C3+, C5+, C7+, and C9+. <i>Chemical Physics Letters</i> , 2002, 363, 486-491.	2.6	18

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19	Competition between Diradical Stepwise and Concerted Mechanisms in Chalcogeno-Diels-Alder Reactions: A Density Functional Study. <i>Journal of Organic Chemistry</i> , 2001, 66, 4026-4035.	3.2	23
20	The correlation of proton affinities with atomic charges and electronegativities for the group 14 to 17 hydrides. <i>Journal of Computational Chemistry</i> , 2000, 21, 1119-1131.	3.3	8
21	Density functional theory predictions for small radicals containing boron and aluminium: broken symmetry problems and solutions. <i>Molecular Physics</i> , 2000, 98, 961-966.	1.7	6
22	Singularities in the behavior of density functionals in predictions of singlet biradicals: The 1,2-dichalcogenins. <i>Journal of Chemical Physics</i> , 2000, 112, 10085-10094.	3.0	20
23	Density functional theory with fractionally occupied frontier orbitals and the instabilities of the Kohn-Sham solutions for defining diradical transition states: Ring-opening reactions. <i>Journal of Chemical Physics</i> , 1999, 111, 7705-7712.	3.0	39
24	Density Functional Study of Systems with Nondynamical Electron Correlation: The S ₃ , Se ₃ , and Te ₃ Potential Energy Surfaces. <i>Journal of Physical Chemistry A</i> , 1999, 103, 4078-4084.	2.5	29
25	Density Functional Study of Tetra-Atomic Clusters and Complexes of the Group 16 Elements: Trends in Structure and Bonding. <i>Journal of Physical Chemistry A</i> , 1999, 103, 6825-6834.	2.5	20
26	Assessment of Basis Set and Functional Dependencies in Density Functional Theory: Studies of Atomization and Reaction Energies. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1927-1934.	2.5	61
27	Ab initio predictions of the structures and spectra of some simple thiosulfeno (XS ₂) free radicals. <i>Journal of Chemical Physics</i> , 1994, 100, 2924-2931.	3.0	18
28	Ab initio studies of the lowest singlet and triplet potential energy surfaces of COS ₂ . <i>Molecular Physics</i> , 1993, 79, 685-697.	1.7	4
29	The COS ₂ potential energy surface: Aspects of the lowest singlet and triplet potential energy surfaces for the reaction of oxygen atoms with carbon disulfide. <i>Journal of Chemical Physics</i> , 1993, 98, 5566-5578.	3.0	7
30	The reaction of sulfur atoms with carbon disulfide: Potential energy surface features. <i>Journal of Chemical Physics</i> , 1992, 96, 7449-7457.	3.0	14
31	Calculated intensity in the local mode overtone spectra of hydrogen peroxide. <i>Journal of Chemical Physics</i> , 1991, 95, 5556-5564.	3.0	38
32	Computational studies of 1,2-dithiete and dithioglyoxal. <i>Journal of Computational Chemistry</i> , 1987, 8, 389-396.	3.3	24
33	Acetaldehyde photochemistry: The radical and molecular dissociations. <i>Journal of Chemical Physics</i> , 1986, 84, 2682-2690.	3.0	86
34	Methoxycarbene and methylhydroxycarbene: Energies, structures, vibrational frequencies, and unimolecular reactivities. <i>Journal of Chemical Physics</i> , 1986, 85, 3975-3984.	3.0	27