John D Goddard

List of Publications by Year
in descending order

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	Ring strain energies: substituted rings, norbornanes, norbornenes and norbornadienes. Tetrahedron, 2004, 60, 8103-8112.	1.9	225
2	Theoretical Study of the Amazing Firefly Bioluminescence:Â The Formation and Structures of the Light Emitters. Journal of the American Chemical Society, 2003, 125, 6962-6971.	13.7	132
3	Acetaldehyde photochemistry: The radical and molecular dissociations. Journal of Chemical Physics, 1986, 84, 2682-2690.	3.0	86
4	Assessment of Basis Set and Functional Dependencies in Density Functional Theory:Â Studies of Atomization and Reaction Energies. Journal of Physical Chemistry A, 1997, 101, 1927-1934.	2.5	61
5	Ruthenium-Catalyzed [2 + 2] Cycloadditions between 7-Substituted Norbornadienes and Alkynes:Â An Experimental and Theoretical Study. Journal of Organic Chemistry, 2004, 69, 8467-8474.	3.2	42
6	Density functional theory with fractionally occupied frontier orbitals and the instabilities of the Kohnâ€“Sham solutions for defining diradical transition states: Ring-opening reactions. Journal of Chemical Physics, 1999, 111, 7705-7712.	3.0	39
7	Calculated intensity in the local mode overtone spectra of hydrogen peroxide. Journal of Chemical Physics, 1991, 95, 5556-5564.	3.0	38
8	Predictions of the Geometries and Fluorescence Emission Energies of Oxyluciferins. Journal of Physical Chemistry A, 2007, 111, 4489-4497.	2.5	37
9	Color-Tuning Mechanism in Firefly Luminescence: Theoretical Studies on Fluorescence of Oxyluciferin in Aqueous Solution Using Time Dependent Density Functional Theory. Journal of Physical Chemistry A, 2008, 112, 9796-9800.	2.5	36
10	A relative approach for determining ring strain energies of heterobicyclic alkenes. Tetrahedron, 2009, 65, 4562-4568.	1.9	35
11	Remote Substituent Effects in Ruthenium-Catalyzed [2+2] Cycloadditions:â€‰ An Experimental and Theoretical Study. Journal of Organic Chemistry, 2006, 71, 3793-3803.	3.2	30
12	Density Functional Study of Systems with Nondynamical Electron Correlation:â€‰ The S3, Se3, and Te3 Potential Energy Surfaces. Journal of Physical Chemistry A, 1999, 103, 4078-4084.	2.5	29
13	Methoxycarbene and methylhydroxycarbene: Energies, structures, vibrational frequencies, and unimolecular reactivities. Journal of Chemical Physics, 1986, 85, 3975-3984.	3.0	27
14	Predictions of the electronic absorption and emission spectra of luciferin and oxyluciferins including solvation effects. Journal of Photochemistry and Photobiology B: Biology, 2005, 81, 163-170.	3.8	25
15	The formation and decomposition of firefly dioxetanone. Chemical Physics Letters, 2011, 506, 269-275.	2.6	25
16	Computational studies of 1,2-dithiete and dithioglyoxal. Journal of Computational Chemistry, 1987, 8, 389-396.	3.3	24
17	Competition between Diradical Stepwise and Concerted Mechanisms in Chalcogeno-Dielsâ€“Alder Reactions:Â A Density Functional Study. Journal of Organic Chemistry, 2001, 66, 4026-4035.	3.2	23
18	Practical failures from the inclusion of exact exchange: how much exact exchange is appropriate?. Molecular Physics, 2002, 100, 483-497.	1.7	22

#	Article	IF	Citations
19	Density Functional Study of Tetra-Atomic Clusters and Complexes of the Group 16 Elements:Â Trends in Structure and Bonding. Journal of Physical Chemistry A, 1999, 103, 6825-6834.	2.5	20
20	Singularities in the behavior of density functionals in predictions of singlet biradicals: The 1,2-dichalcogenins. Journal of Chemical Physics, 2000, 112, 10085-10094.	3.0	20
21	Ab initio predictions of the structures and spectra of some simple thiosulfeno (XS2) free radicals. Journal of Chemical Physics, 1994, 100, 2924-2931.	3.0	18
22	Is density functional theory free of spatial symmetry breaking? The case of the linear carbon radical cations: C3+, C5+, C7+, and C9+. Chemical Physics Letters, 2002, 363, 486-491.	2.6	18
23	Ruthenium-catalyzed [2+2] cycloadditions between substituted alkynes and norbornadiene: a theoretical study. Tetrahedron, 2007, 63, 7659-7666.	1.9	16
24	Assessment of density functional theory for the prediction of the nature of the oxirene stationary point. Computational and Theoretical Chemistry, 2003, 629, 263-270.	1.5	15
25	The Spectralâ€“Structural Relationship of a Series of Oxyluciferin Derivatives. ChemPhysChem, 2015, 16, 396-402.	2.1	15
26	The reaction of sulfur atoms with carbon disulfide: Potential energy surface features. Journal of Chemical Physics, 1992, 96, 7449-7457.	3.0	14
27	The correlation of proton affinities with atomic charges and electronegativities for the group 14 to 17 hydrides. Journal of Computational Chemistry, 2000, 21, 1119-1131.	3.3	8
28	The COS2potential energy surface: Aspects of the lowest singlet and triplet potential energy surfaces for the reaction of oxygen atoms with carbon disulfide. Journal of Chemical Physics, 1993, 98, 5566-5578.	3.0	7
29	Density functional theory predictions for small radicals containing boron and aluminium: broken symmetry problems and solutions. Molecular Physics, 2000, 98, 961-966.	1.7	6
30	Ab initio studies of the lowest singlet and triplet potential energy surfaces of CO2S. Molecular Physics, 1993, 79, 685-697.	1.7	4
31	Consequences of accidental degeneracy within density functional theory: the enigmatic structure of boron nitrosyl. Chemical Physics Letters, 2002, 356, 7-13.	2.6	2
32	Effect of Explicit Water Molecules on the Colorâ€Tuning Mechanism of the Firefly. Chinese Journal of Chemistry, 2011, 29, 2301-2307.	4.9	2
33	Electronic and optical properties of the five most stable C96 isomers. Chemical Physics Letters, 2015, 625, 64-68.	2.6	1
34	Theoretical studies of the structural, electronic, and ¹⁹F NMR properties of linear and branched perfluorobutanesulfonate. Canadian Journal of Chemistry, 2013, 91, 1272-1280.	1.1	0