Eric Jon Sundstrom

List of Publications by Year in descending order

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759055 1125617 3,623 12 12 13 citations h-index g-index papers 13 13 13 4460 docs citations times ranked citing authors all docs

#	Article	IF	CITATIONS
1	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
2	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
3	LOBA: a localized orbital bonding analysis to calculate oxidation states, with application to a model water oxidation catalyst. Physical Chemistry Chemical Physics, 2009, 11, 11297.	1.3	134
4	Unrestricted absolutely localized molecular orbitals for energy decomposition analysis: Theory and applications to intermolecular interactions involving radicals. Journal of Chemical Physics, 2013, 138, 134119.	1.2	90
5	Computational and Experimental Study of the Mechanism of Hydrogen Generation from Water by a Molecular Molybdenum-Oxo Electrocatalyst. Journal of the American Chemical Society, 2012, 134, 5233-5242.	6.6	68
6	Non-orthogonal configuration interaction for the calculation of multielectron excited states. Journal of Chemical Physics, 2014, 140, 114103.	1.2	66
7	Useful lower limits to polarization contributions to intermolecular interactions using a minimal basis of localized orthogonal orbitals: Theory and analysis of the water dimer. Journal of Chemical Physics, 2013, 138, 084102.	1.2	38
8	Spin–flip non-orthogonal configuration interaction: a variational and almost black-box method for describing strongly correlated molecules. Physical Chemistry Chemical Physics, 2014, 16, 22694-22705.	1.3	38
9	Degree of Initial Hole Localization/Delocalization in Ionized Water Clusters. Journal of Physical Chemistry A, 2009, 113, 4423-4429.	1.1	35
10	Wavefunction stability analysis without analytical electronic Hessians: application to orbital-optimised second-order MÃ,ller–Plesset theory and W10-containing density functionals. Molecular Physics, 2015, 113, 1802-1808.	0.8	30
11	Restricted Hartree Fock using complex-valued orbitals: A long-known but neglected tool in electronic structure theory. Journal of Chemical Physics, 2015, 142, 024104.	1.2	26
12	A simple way to test for collinearity in spin symmetry broken wave functions: General theory and application to generalized Hartree Fock. Journal of Chemical Physics, 2015, 142, 094112.	1.2	16