Robert Balawender

List of Publications by Year
in descending order

22 papers	503 citations	623734 14 h-index	839539 18 g-index
22 all docs	22 docs citations	22 times ranked	366 citing authors

#	Article	IF	Citations
1	Atomic Fukui function indices and local softness ab initio. Journal of Chemical Physics, 1998, 109, 5203-5211.	3.0	73
2	Exploring Chemical Space with the Alchemical Derivatives. Journal of Chemical Theory and Computation, 2013, 9, 5327-5340.	5.3	42
3	Nuclear Fukui function from coupled perturbed Hartreeâ€“Fock equations. Journal of Chemical Physics, 2001, 114, 682.	3.0	40
4	Derivatives of Molecular Valence as a Measure of Aromaticity. Journal of Physical Chemistry A, 1998, 102, 9912-9917.	2.5	36
5	Nuclear Fukui function and Berlinâ€™s binding function: Prediction of the Jahnâ€“Teller distortion. Journal of Chemical Physics, 2001, 114, 4441.	3.0	36
6	Revisiting the chemical reactivity indices as the state function derivatives. The role of classical chemical hardness. Journal of Chemical Physics, 2015, 142, 054104.	3.0	32
7	Solvent Effect on the Global and Atomic DFT-Based Reactivity Descriptors Using the Effective Fragment Potential Model. Solvation of Ammonia. Journal of Physical Chemistry A, 2001, 105, 6703-6710.	2.5	31
8	Higher order alchemical derivatives from coupled perturbed self-consistent field theory. Journal of Chemical Physics, 2012, 136, 034104.	3.0	31
9	Exploring Chemical Space with Alchemical Derivatives: BN-Simultaneous Substitution Patterns in C₆₀. Journal of Chemical Theory and Computation, 2018, 14, 1154-1168.	5.3	31
10	Solvent Effect on Electronegativity, Hardness, Condensed Fukui Functions, and Softness, in a Large Series of Diatomic and Small Polyatomic Molecules:â€‰ Use of the EFP Model. Journal of Physical Chemistry A, 2001, 105, 11102-11109.	2.5	25
11	DFT-based chemical reactivity indices in the Hartree-Fock method. II. Fukui function, chemical potential, and hardness. Journal of Chemical Physics, 2005, 123, 124103.	3.0	22
12	Acidic and basic molecular hardness in LCAO approximation. International Journal of Quantum Chemistry, 1997, 61, 499-505.	2.0	19
13	Exploring chemical space with alchemical derivatives: alchemical transformations of H through Ar and their ions as a proof of concept. Physical Chemistry Chemical Physics, 2019, 21, 23865-23879.	2.8	19
14	Density-functional theory-based chemical reactivity indices in the Hartree-Fock method. I. Unrestricted Hartree-Fock method for a noninteger number of electrons. Journal of Chemical Physics, 2005, 123, 124102.	3.0	16
15	Comment on â€œLegendre-transform functionals for spin-density-functional theoryâ€•[J. Chem. Phys. 124, 224108 (2006)]. Journal of Chemical Physics, 2006, 125, 247101.	3.0	14
16	Structure Investigations of Dichloroaluminum Benzoates: An Unprecedented Example of a Monomeric Aluminum Complex with a Chelating Carboxylate Ligand. Inorganic Chemistry, 2009, 48, 10892-10894.	4.0	14
17	THE NUCLEAR FUKUI FUNCTION. , 2002, , 1053-1070.		7
18	Information and complexity measures in molecular reactivity studies. Physical Chemistry Chemical Physics, 2014, 16, 14928-14946.	2.8	6

#	Article	IF	Citations
19	Alchemical Derivatives of Atoms: A Walk Through the Periodic Table. , 2018, , 227-251.		4
20	New Insights and Horizons from the Linear Response Function in Conceptual DFT. , 0, , .		3
21	Testing exchangeâ€“correlation functionals at fractional electron numbers. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	2
22	Acidic and basic molecular hardness in LCAO approximation. International Journal of Quantum Chemistry, 1997, 61, 499-505.	2.0	0