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	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
2	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
3	Alchemical Derivatives of Atoms: A Walk Through the Periodic Table. , 2018, , 227-251.		4
4	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
5	Information and complexity measures in molecular reactivity studies. Physical Chemistry Chemical Physics, 2014, 16, 14928-14946.	2.8	6
6	Testing exchangeâ€“correlation functionals at fractional electron numbers. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	2
7	Exploring Chemical Space with the Alchemical Derivatives. Journal of Chemical Theory and Computation, 2013, 9, 5327-5340.	5.3	42
8	Higher order alchemical derivatives from coupled perturbed self-consistent field theory. Journal of Chemical Physics, 2012, 136, 034104.	3.0	31
9	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
10	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
11	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
12	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
13	THE NUCLEAR FUKUI FUNCTION. , 2002, , 1053-1070.		7
14	Nuclear Fukui function from coupled perturbed Hartreeâ€“Fock equations. Journal of Chemical Physics, 2001, 114, 682.	3.0	40
15	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
16	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
17	Nuclear Fukui function and Berlinâ€™s binding function: Prediction of the Jahnâ€“Teller distortion. Journal of Chemical Physics, 2001, 114, 4441.	3.0	36
18	Atomic Fukui function indices and local softness ab initio. Journal of Chemical Physics, 1998, 109, 5203-5211.	3.0	73

#	Article	IF	Citations
19	Derivatives of Molecular Valence as a Measure of Aromaticity. Journal of Physical Chemistry A, 1998, 102, 9912-9917.	2.5	36
20	Acidic and basic molecular hardness in LCAO approximation. International Journal of Quantum Chemistry, 1997, 61, 499-505.	2.0	19
21	Acidic and basic molecular hardness in LCAO approximation. International Journal of Quantum Chemistry, 1997, 61, 499-505.	2.0	0
22	New Insights and Horizons from the Linear Response Function in Conceptual DFT. , 0, , .		3