Junia Melin

List of Publications by Year
in descending order

16	827	758635 12	940134 16
papers	citations	h-index	g-index

16	16	16	590
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Using the general-purpose reactivity indicator: challenging examples. Journal of Molecular Modeling, 2016, 22, 57.	0.8	5
2	Efficient evaluation of analytic Fukui functions. Journal of Chemical Physics, 2008, 129, 224105.	1.2	60
3	Chapter 6 Electronic structure and reactivity in double Rydberg anions: characterization of a novel kind of electron pair. Theoretical and Computational Chemistry, 2007, 19, 87-100.	0.2	10
4	O H 3 â^' and O2H5â^' double Rydberg anions: Predictions and comparisons with NH4â^' and N2H7â^'. Journal of Chemical Physics, 2007, 127, 014307.	1.2	16
5	Removing Electrons Can Increase the Electron Density:Â A Computational Study of Negative Fukui Functions. Journal of Physical Chemistry A, 2007, 111, 10017-10019.	1.1	105
6	Further links between the maximum hardness principle and the hard/soft acid/base principle: insights from hard/soft exchange reactions. Physical Chemistry Chemical Physics, 2007, 9, 3853.	1.3	89
7	Tautomeric Forms of Azolide Anions:Â Vertical Electron Detachment Energies and Dyson Orbitals. Journal of Physical Chemistry A, 2007, 111, 13069-13074.	1.1	10
8	Conceptual Density-Functional Theory for General Chemical Reactions, Including Those That Are Neither Charge- nor Frontier-Orbital-Controlled. 2. Application to Molecules Where Frontier Molecular Orbital Theory Fails. Journal of Chemical Theory and Computation, 2007, 3, 375-389.	2.3	98
9	Conceptual Density-Functional Theory for General Chemical Reactions, Including Those That Are Neither Charge- nor Frontier-Orbital-Controlled. 1. Theory and Derivation of a General-Purpose Reactivity Indicator. Journal of Chemical Theory and Computation, 2007, 3, 358-374.	2.3	141
10	Computing the Fukui function from ab initio quantum chemistry: approaches based on the extended Koopmansâ€™ theorem. Theoretical Chemistry Accounts, 2007, 117, 371-381.	0.5	35
11	Electronic Structure Analysis and Electron Detachment Energies of Polynitrogen Pentagonal Aromatic Anions. Journal of Physical Chemistry A, 2006, 110, 12231-12235.	1.1	12
12	The electron-propagator approach to conceptual density-functional theory. Journal of Chemical Sciences, 2005, 117, 387-400.	0.7	33
13	Ground and excited states of the Rydberg radical H3O: Electron propagator and quantum defect analysis. Journal of Chemical Physics, 2005, 122, 234317.	1.2	14
14	Is the Fukui Function a Right Descriptor of Hardâ^'Hard Interactions?. Journal of Physical Chemistry A, 2004, 108, 2487-2491.	1.1	131
15	Application of the electron localization function to radical systems. International Journal of Quantum Chemistry, 2003, 92, 381-390.	1.0	39
16	Chemical Reactivity in the {N, NS, v(r)} Space. Journal of Physical Chemistry A, 2003, 107, 3831-3835.	1.1	29