Andres Cedillo

List of Publications by Year
in descending order

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49 papers	1,658 citations	430754 18 h-index	289141 40 g-index
50 all docs	50 docs citations	50 times ranked	1239 citing authors

#	Article	IF	Citations
1	Electrodonating and Electroaccepting Powers. Journal of Physical Chemistry A, 2007, 111, 1966-1970.	1.1	540
2	Variational method for determining the Fukui function and chemical hardness of an electronic system. Journal of Chemical Physics, 1995, 103, 7645-7646.	1.2	138
3	Fukui function from a gradient expansion formula, and estimate of hardness and covalent radius for an atom. Journal of Chemical Physics, 1995, 103, 10621-10626.	1.2	89
4	Reactivity indices and fluctuation formulas in density functional theory: Isomorphic ensembles and a new measure of local hardness. Journal of Chemical Physics, 1995, 103, 8548-8556.	1.2	88
5	Reactivity indicators for degenerate states in the density-functional theoretic chemical reactivity theory. Journal of Chemical Physics, 2011, 134, 174103.	1.2	74
6	Appraisal of Chemical Bond Making, Bond Breaking, and Electron Transfer in Solution in the Light of the Principle of Maximum Hardness. Journal of Organic Chemistry, 1995, 60, 4707-4714.	1.7	65
7	Nucleophilicity Index from Perturbed Electrostatic Potentials. Journal of Physical Chemistry A, 2007, 111, 2442-2447.	1.1	59
8	Atoms-in-molecules partitioning of a molecular density. International Journal of Quantum Chemistry, 2000, 77, 403-407.	1.0	58
9	Chemical softness in model electronic systems: dependence on temperature and chemical potential. Chemical Physics, 1996, 204, 429-437.	0.9	57
10	Comparison between the frozen core and finite differences approximations for the generalized spin-dependent global and local reactivity descriptors in small molecules. Theoretical Chemistry Accounts, 2006, 115, 257-265.	0.5	53
11	Koopmans-like Approximation in the Kohnâ^'Sham Method and the Impact of the Frozen Core Approximation on the Computation of the Reactivity Parameters of the Density Functional Theory. Journal of Physical Chemistry A, 2005, 109, 8880-8892.	1.1	44
12	The variations of the hardness and the Kohnâ€“Sham Fukui function under an external perturbation. Journal of Chemical Physics, 1999, 110, 9807-9811.	1.2	35
13	The Markovnikov Regioselectivity Rule in the Light of Site Activation Models. Journal of Physical Chemistry A, 2002, 106, 7844-7849.	1.1	31
14	A new representation for ground states and its legendre transforms. International Journal of Quantum Chemistry, 1994, 52, 231-240.	1.0	29
15	Gas phase Lewis acidity and basicity scales for boranes, phosphines and amines based on the formation of donorâ€“acceptor complexes. Computational and Theoretical Chemistry, 2013, 1011, 44-56.	1.1	29
16	A perturbative approach to the Thomasâ€“Fermi equation in terms of the density. Journal of Mathematical Physics, 1993, 34, 2713-2717.	0.5	27
17	REACTIVITY CRITERIA IN SPIN-POLARIZED DENSITY FUNCTIONAL THEORY. , 2002, , 936-965.		25
18	Quantum Mechanical Tunneling through Barriers: A Spreadsheet Approach. Journal of Chemical Education, 2000, 77, 528.	1.1	20

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19	Charge transfer and adsorption energies in the iodineâ€“Pt(111) interaction. Surface Science, 2005, 581, 58-65.	0.8	20
20	New nonlocal exchange-energy functional from a kinetic-energy-density PadÃ©-approximant model. Physical Review A, 1988, 38, 1697-1701.	1.0	19
21	Global and Local Reactivity and Activation Patterns of HOOX (X = H, NO2, CO2-, SO3-) Peroxides with Solvent Effects. Journal of Physical Chemistry A, 2003, 107, 10098-10104.	1.1	16
22	Bond fukui indices: Comparison of frozen molecular orbital and finite differences through mulliken populations. Journal of Computational Chemistry, 2013, 34, 2421-2429.	1.5	14
23	On the Existence of Electronic States Confined by Charged Groups in Proteins. Journal of Physical Chemistry B, 2003, 107, 1692-1697.	1.2	13
24	Solvent effects on the energetic parameters and chemical reactivity in the ketoâ€“enol tautomeric equilibrium of substituted carbonyl compounds. Computational and Theoretical Chemistry, 2012, 994, 47-53.	1.1	11
25	Self-consistent methods constrained to a fixed number of particles in a given fragment and its relation to the electronegativity equalization method. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	11
26	HÃ¼ckelâ€type semiempirical implementation of a variational method for determining electronic band gaps. Journal of Chemical Physics, 1996, 105, 9557-9560.	1.2	10
27	Stability of the different AlOOH phases under pressure. Journal of Physics Condensed Matter, 2016, 28, 185401.	0.7	10
28	Performance of density functional theory methods to describe intramolecular hydrogen shifts. Journal of Chemical Sciences, 2005, 117, 555-560.	0.7	9
29	Molecular Fragments in Density Functional Theory. Journal of Physical Chemistry A, 2006, 110, 4535-4537.	1.1	9
30	Wave function instabilities in the cisâ€“trans isomerization and singletâ€“triplet energy gaps in a pushâ€“pull compound. Journal of Chemical Physics, 2003, 119, 4112-4116.	1.2	7
31	An exchange energy functional based on the Dirac and the Fermiâ€“Amaldi approximations. Journal of Chemical Physics, 1986, 85, 7188-7192.	1.2	6
32	Br2 dissociation in water clusters: the catalytic role of water. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	5
33	Interatomic interactions in density functional theory. International Journal of Quantum Chemistry, 1986, 29, 937-948.	1.0	4
34	On the Principle of Spin Potential Equalization. Journal of Physical Chemistry A, 2009, 113, 1390-1396.	1.1	4
35	The density response kernel, the Fukui function, and other response functions from the Kohnâ€“Sham orbitals. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	4
36	Softâ€“Soft interactions in the proteinâ€“protein recognition process: The K⁺ channelâ€charybdotoxin case. International Journal of Quantum Chemistry, 2012, 112, 3618-3623.	1.0	3

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37	Chemical reactivity of the frustrated Lewis pairs in borophosphines: a theoretical analysis of their Lewis acidity, Lewis basicity and Fukui function. Journal of Molecular Modeling, 2018, 24, 238.	0.8	3
38	Reactivity of Carbon Molecular Clusters from a HÃ¼ckel-Type Model. Journal of Physical Chemistry A, 2019, 123, 8696-8701.	1.1	3
39	Shape Function. , 2009, , .		3
40	Theoretical estimation of the electron affinity of enolate radicals. International Journal of Quantum Chemistry, 2009, 109, 1031-1035.	1.0	2
41	Comment on â€œPower Law Distribution Concerning Absolute Free Energies of Linear Sulfur Chains, Polythiazyls, Polyisoprenes, Linear trans-Polyenes, and Polyynesâ€• Journal of Physical Chemistry A, 2019, 123, 7540-7541.	1.1	2
42	The Role of the Density Response Kernel in the Protonation Process. Journal of Physical Chemistry A, 2020, 124, 858-863.	1.1	2
43	Chapter 2 Density functional theory models of reactivity based on an energetic criterion. Theoretical and Computational Chemistry, 2007, 19, 19-30.	0.2	1
44	Stability and bonding in the boraneâ€“H₂ complexes. International Journal of Quantum Chemistry, 2012, 112, 3564-3569.	1.0	1
45	Comment on â€œLocalizationâ€“delocalization phenomena in a cyclic boxâ€• by H. H. Corzo, H. G. Laguna, and R. P. Sagar. Journal of Mathematical Chemistry, 2017, 55, 1889-1892.	0.7	1
46	Prediction of the tautomer stability and acidity of phenacylpyridines in aqueous solution. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	1
47	A Local Extension of the Electrophilicity Index Concept. Journal of the Mexican Chemical Society, 2017, 56, .	0.2	1
48	Prediction of the solidâ€“solid pressure-induced phase transition in cubic ionic crystals with empirical potentials. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	0
49	Structural Phase Transitions in Cesium Halides. , 1991, , 293-306.		0