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	Prediction of the tautomer stability and acidity of phenacylpyridines in aqueous solution. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	1
2	The Role of the Density Response Kernel in the Protonation Process. Journal of Physical Chemistry A, 2020, 124, 858-863.	1.1	2
3	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
4	Reactivity of Carbon Molecular Clusters from a HÃ¼ckel-Type Model. Journal of Physical Chemistry A, 2019, 123, 8696-8701.	1.1	3
5	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
6	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
7	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
8	A Local Extension of the Electrophilicity Index Concept. Journal of the Mexican Chemical Society, 2017, 56, .	0.2	1
9	Stability of the different AlOOH phases under pressure. Journal of Physics Condensed Matter, 2016, 28, 185401.	0.7	10
10	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
11	Br2 dissociation in water clusters: the catalytic role of water. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	5
12	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
13	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
14	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
15	Stability and bonding in the boraneâ€“H₂ complexes. International Journal of Quantum Chemistry, 2012, 112, 3564-3569.	1.0	1
16	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
17	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
18	Reactivity indicators for degenerate states in the density-functional theoretic chemical reactivity theory. Journal of Chemical Physics, 2011, 134, 174103.	1.2	74

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19	Theoretical estimation of the electron affinity of enolate radicals. International Journal of Quantum Chemistry, 2009, 109, 1031-1035.	1.0	2
20	On the Principle of Spin Potential Equalization. Journal of Physical Chemistry A, 2009, 113, 1390-1396.	1.1	4
21	Shape Function. , 2009, , .		3
22	Nucleophilicity Index from Perturbed Electrostatic Potentials. Journal of Physical Chemistry A, 2007, 111, 2442-2447.	1.1	59
23	Electrodonating and Electroaccepting Powers. Journal of Physical Chemistry A, 2007, 111, 1966-1970.	1.1	540
24	Chapter 2 Density functional theory models of reactivity based on an energetic criterion. Theoretical and Computational Chemistry, 2007, 19, 19-30.	0.2	1
25	Molecular Fragments in Density Functional Theory. Journal of Physical Chemistry A, 2006, 110, 4535-4537.	1.1	9
26	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
27	Charge transfer and adsorption energies in the iodineâ€“Pt(111) interaction. Surface Science, 2005, 581, 58-65.	0.8	20
28	Performance of density functional theory methods to describe intramolecular hydrogen shifts. Journal of Chemical Sciences, 2005, 117, 555-560.	0.7	9
29	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
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	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
32	On the Existence of Electronic States Confined by Charged Groups in Proteins. Journal of Physical Chemistry B, 2003, 107, 1692-1697.	1.2	13
33	The Markovnikov Regioselectivity Rule in the Light of Site Activation Models. Journal of Physical Chemistry A, 2002, 106, 7844-7849.	1.1	31
34	REACTIVITY CRITERIA IN SPIN-POLARIZED DENSITY FUNCTIONAL THEORY. , 2002, , 936-965.		25
35	Atoms-in-molecules partitioning of a molecular density. International Journal of Quantum Chemistry, 2000, 77, 403-407.	1.0	58
36	Quantum Mechanical Tunneling through Barriers: A Spreadsheet Approach. Journal of Chemical Education, 2000, 77, 528.	1.1	20

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37	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
38	HÃ¼ckelâ€type semiempirical implementation of a variational method for determining electronic band gaps. Journal of Chemical Physics, 1996, 105, 9557-9560.	1.2	10
39	Chemical softness in model electronic systems: dependence on temperature and chemical potential. Chemical Physics, 1996, 204, 429-437.	0.9	57
40	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
41	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
42	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
43	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
44	A new representation for ground states and its legendre transforms. International Journal of Quantum Chemistry, 1994, 52, 231-240.	1.0	29
45	A perturbative approach to the Thomasâ€“Fermi equation in terms of the density. Journal of Mathematical Physics, 1993, 34, 2713-2717.	0.5	27
46	Structural Phase Transitions in Cesium Halides. , 1991, , 293-306.		0
47	New nonlocal exchange-energy functional from a kinetic-energy-density PadÃ©-approximant model. Physical Review A, 1988, 38, 1697-1701.	1.0	19
48	Interatomic interactions in density functional theory. International Journal of Quantum Chemistry, 1986, 29, 937-948.	1.0	4
49	An exchange energy functional based on the Dirac and the Fermiâ€“Amaldi approximations. Journal of Chemical Physics, 1986, 85, 7188-7192.	1.2	6