Carlos Cardenas

List of Publications by Year
in descending order

72 papers	1,550 citations	279798 23 h-index	345221 36 g-index
75 all docs	75 docs citations	75 times ranked	981 citing authors

#	Article	IF	Citations
1	Chemical Reactivity Descriptors for Ambiphilic Reagents: Dual Descriptor, Local Hypersoftness, and Electrostatic Potential. Journal of Physical Chemistry A, 2009, 113, 8660-8667.	2.5	166
2	Reactivity indicators for degenerate states in the density-functional theoretic chemical reactivity theory. Journal of Chemical Physics, 2011, 134, 174103.	3.0	74
3	Should negative electron affinities be used for evaluating the chemical hardness?. Physical Chemistry Chemical Physics, 2011, 13, 2285-2293.	2.8	69
4	Proposal of a simple and effective local reactivity descriptor through a topological analysis of an orbitalâ€weighted fukui function. Journal of Computational Chemistry, 2017, 38, 481-488.	3.3	58
5	The Fukui Potential and the Capacity of Charge and the Global Hardness of Atoms. Journal of Physical Chemistry A, 2011, 115, 2325-2331.	2.5	56
6	How to Compute the Fukui Matrix and Function for Systems with (Quasi-)Degenerate States. Journal of Chemical Theory and Computation, 2014, 10, 202-210.	5.3	53
7	Benchmark values of chemical potential and chemical hardness for atoms and atomic ions (including) Tj ETQq1 1 0.784314 rgBT /Ove 18, 25721-25734.	2.8	51
8	Atomic Charges and the Electrostatic Potential Are Ill-Defined in Degenerate Ground States. Journal of Chemical Theory and Computation, 2013, 9, 4779-4788.	5.3	48
9	An explicit approach to conceptual density functional theory descriptors of arbitrary order. Chemical Physics Letters, 2016, 660, 307-312.	2.6	46
10	How reliable is the hardâ€“soft acidâ€“base principle? An assessment from numerical simulations of electron transfer energies. Physical Chemistry Chemical Physics, 2013, 15, 13959.	2.8	44
11	In pursuit of negative Fukui functions: examples where the highest occupied molecular orbital fails to dominate the chemical reactivity. Journal of Molecular Modeling, 2013, 19, 2779-2783.	1.8	43
12	Relationships between the third-order reactivity indicators in chemical density-functional theory. Journal of Chemical Physics, 2009, 130, 244105.	3.0	35
13	The Fukui potential is a measure of the chemical hardness. Chemical Physics Letters, 2011, 513, 127-129.	2.6	34
14	An information-theoretic resolution of the ambiguity in the local hardness. Physical Chemistry Chemical Physics, 2014, 16, 6019-6026.	2.8	34
15	How predictive could alchemical derivatives be?. Physical Chemistry Chemical Physics, 2017, 19, 16003-16012.	2.8	34
16	Theoretical study of the surface reactivity of alkaline earth oxides: Local density of states evaluation of the local softness. Journal of Chemical Physics, 2008, 128, 034708.	3.0	31
17	Communication: A case where the hard/soft acid/base principle holds regardless of acid/base strength. Journal of Chemical Physics, 2013, 138, 181106.	3.0	31
18	Density functional theory of chemical reactivity. Chemical Modelling, 2014, , 151-174.	0.4	30

#	Article	IF	Citations
19	On the exponential model for energy with respect to number of electrons. Journal of Molecular Modeling, 2013, 19, 2849-2853.	1.8	29
20	The HSAB principle from a finite-temperature grand-canonical perspective. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	28
21	Further exploration of the Fukui function, hardness, and other reactivity indices and its relationships within the Kohnâ€“Sham scheme. International Journal of Quantum Chemistry, 2007, 107, 37-45.	2.0	27
22	Magnon valley Hall effect in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>CrI</mml:mi></mml:mrow><mml:mn>3</mml:mn> -based van der Waals heterostructures. Physical Review B, 2020, 101, .	3.2	26
23	Hematene: a 2D magnetic material in van der Waals or non-van der Waals heterostructures. 2D Materials, 2019, 6, 045002.	4.4	24
24	Nature of Bonding in the Cyclization Reactions of (2-Ethynylphenyl)triazene and 2-Ethynylstyrene. Journal of Physical Chemistry A, 2005, 109, 4352-4358.	2.5	23
25	Symmetric Nonlocal Weighted Density Approximations from the Exchange-Correlation Hole of the Uniform Electron Gas. Journal of Chemical Theory and Computation, 2012, 8, 4081-4093.	5.3	22
26	In pursuit of negative Fukui functions: molecules with very small band gaps. Journal of Molecular Modeling, 2014, 20, 2162.	1.8	22
27	Local electrophilicity. Journal of Molecular Modeling, 2018, 24, 245.	1.8	21
28	Assembling Small Silicon Clusters Using Criteria of Maximum Matching of the Fukui Functions. Journal of Chemical Theory and Computation, 2011, 7, 3995-4001.	5.3	20
29	Computing the Fukui Function in Solid-State Chemistry: Application to Alkaline Earth Oxides Bulk and Surfaces. Journal of Physical Chemistry A, 2020, 124, 2826-2833.	2.5	20
30	Topological Analysis of the Fukui Function. Challenges and Advances in Computational Chemistry and Physics, 2016, , 227-241.	0.6	19
31	Mechanism of fluorophore quenching in a pre-fluorescent nitroxide probe: A theoretical illustration. Chemical Physics Letters, 2014, 593, 89-92.	2.6	18
32	Nuclear reactivity indices in the context of spin polarized density functional theory. Chemical Physics, 2006, 322, 303-310.	1.9	16
33	A chemical theory of topological insulators. Chemical Communications, 2019, 55, 12281-12287.	4.1	16
34	A problematic issue for atoms in molecules: Impact of (quasi-)degenerate states on Quantum Theory Atoms in Molecules and Hirshfeld-I properties. Computational and Theoretical Chemistry, 2015, 1053, 106-111.	2.5	15
35	Regional Electrophilic and Nucleophilic Fukui Functions Efficiently Highlight the Lewis Acidic/Basic Regions in Ionic Liquids. Journal of Physical Chemistry B, 2014, 118, 3696-3701.	2.6	14
36	Electron Localization Function in Excited States: The Case of the Ultrafast Proton Transfer of the Salicylidene Methylamine. Journal of Chemical Theory and Computation, 2019, 15, 5532-5542.	5.3	14

#	Article	IF	Citations
37	Kickâ€“Fukui: A Fukui Function-Guided Method for Molecular Structure Prediction. Journal of Chemical Information and Modeling, 2021, 61, 3955-3963.	5.4	14
38	Condensation of the highest occupied molecular orbital within the electron localization function domains. Journal of Chemical Sciences, 2005, 117, 419-424.	1.5	13
39	Predicting Deprotonation Sites Using Alchemical Derivatives. Journal of Physical Chemistry A, 2020, 124, 3754-3760.	2.5	13
40	On the Prediction of Lattice Energy with the Fukui Potential: Some Supports on Hardness Maximization in Inorganic Solids. Journal of Physical Chemistry A, 2022, 126, 4507-4516.	2.5	13
41	Theoretical Study on CDK2 Inhibitors Using a Global Softness Obtained from the Density of States. Journal of Physical Chemistry B, 2007, 111, 3293-3297.	2.6	12
42	Nuclear Fukui functions from nonintegral electron number calculations. International Journal of Quantum Chemistry, 2007, 107, 807-815.	2.0	11
43	Understanding chemical binding using the Berlin function and the reaction force. Chemical Physics Letters, 2012, 539-540, 168-171.	2.6	11
44	A theoretical study of the photodynamics of salicylidene-2-anthrylamine in acetonitrile solution. Physical Chemistry Chemical Physics, 2018, 20, 29399-29411.	2.8	10
45	Links among the Fukui potential, the alchemical hardness and the local hardness of an atom in a molecule. Journal of Computational Chemistry, 2021, 42, 1681-1688.	3.3	10
46	On the nature of bonding in the photochemical addition of two ethylenes: Câ€“C bond formation in the excited state?. Physical Chemistry Chemical Physics, 2021, 23, 20598-20606.	2.8	10
47	On understanding the chemical origin of band gaps. Journal of Molecular Modeling, 2017, 23, 271.	1.8	9
48	The Pauli principle and the confinement of electron pairs in a double well: Aspects of electronic bonding under pressure. Journal of Chemical Physics, 2019, 150, 204304.	3.0	9
49	Theoretical analysis of the adsorption of ammoniaâ€“borane and their dehydrogenation products on the (001) surface of TiC and ZrC. Surface Science, 2019, 680, 95-106.	1.9	9
50	On the recognition of chloride, bromide and nitrate anions by anthraceneâ€“squaramide conjugated compounds: a computational perspective. New Journal of Chemistry, 2020, 44, 17831-17839.	2.8	9
51	Performance of modified Lennardâ€“Jones potential to seed ab initio calculations of small cadmium clusters. Computational and Theoretical Chemistry, 2013, 1021, 249-255.	2.5	8
52	Ab Initio Molecular Dynamics Study of Small Alkali Metal Clusters. Journal of Physical Chemistry A, 2014, 118, 1077-1083.	2.5	8
53	Molecular simulations of carbon allotropes in processes with creation and destruction of chemical bonds. Carbon, 2019, 144, 177-184.	10.3	8
54	Negative Condensed-to-Atom Fukui Functions: A Signature of Oxidation-Induced Reduction of Functional Groups. , 2017, , 269-278.		7

#	Article	IF	Citations
55	Formation of complex organic molecules in ice mantles: An ab initio molecular dynamics study. Astronomy and Astrophysics, 2019, 629, A28.	5.1	7
56	Orbital energies and nuclear forces in <scp>DFT</scp>: Interpretation and validation. Journal of Computational Chemistry, 2021, 42, 334-343.	3.3	7
57	A new isomer of C20 and a way to a new C240. Physical Chemistry Chemical Physics, 2012, 14, 14810.	2.8	6
58	Electronic structure of first and second row atoms under harmonic confinement. International Journal of Quantum Chemistry, 2020, 120, e26132.	2.0	6
59	Molecular Interactions From the Density Functional Theory for Chemical Reactivity: The Interaction Energy Between Two-Reagents. Frontiers in Chemistry, 0, 10, .	3.6	6
60	Interaction of Nitroxide Radicals with an Au₈ Nanostructure: Theoretical and Calorimetric Studies. Journal of Physical Chemistry C, 2019, 123, 21713-21720.	3.1	4
61	Ferromagnetic bond of Li10 cluster: An alternative approach in terms of effective ferromagnetic sites. Journal of Chemical Physics, 2016, 145, 094301.	3.0	3
62	Reactivity of Carbon Molecular Clusters from a HÃ¼ckel-Type Model. Journal of Physical Chemistry A, 2019, 123, 8696-8701.	2.5	3
63	The change in the nature of bonding in the Li 2 dimer under confinement. International Journal of Quantum Chemistry, 2021, 121, e26644.	2.0	3
64	Electronegativity under Confinement. Molecules, 2021, 26, 6924.	3.8	2
65	Ab Initio Molecular Dynamics Simulations of Ti₂ on C₂₀ Collisions and C₂₀Ti₂ Configurations. Journal of Physical Chemistry C, 2013, 117, 4287-4291.	3.1	1
66	Reaction channels and spectroscopic constants of astrophysical relevant Silicon bearing molecules SiC3H,+ and SiC3H. Monthly Notices of the Royal Astronomical Society, 2014, 443, 3127-3133.	4.4	1
67	Coulomb Explosion of Multi-charged Atomic Alkaline Metal Clusters. Journal of Physical Chemistry A, 2021, 125, 2512-2517.	2.5	1
68	Understanding Topological Insulators in Real Space. Molecules, 2021, 26, 2965.	3.8	1
69	Cluster Assembled Silicon-Lithium Nanostructures: A Nanowire Confined Inside a Carbon Nanotube. Frontiers in Chemistry, 2021, 9, 767421.	3.6	1
70	A numerical study of the Liebâ€“Thirring kinetic energy lower bound. Molecular Physics, 2016, 114, 982-987.	1.7	0
71	On the chemical potential of the hydrogen atom. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	0
72	Designing boron and metal complexes for fluoride recognition: a computational perspective. Physical Chemistry Chemical Physics, 2021, 23, 22768-22778.	2.8	0