Alberto Vela

List of Publications by Year
in descending order

121 papers	5,292 citations	94269 37 h-index	91712 69 g-index
129 all docs	129 docs citations	129 times ranked	3818 citing authors

#	Article	IF	Citations
1	Electrodonating and Electroaccepting Powers. Journal of Physical Chemistry A, 2007, 111, 1966-1970.	1.1	540
2	Quantum Chemical Study of the Inhibitive Properties of 2-Pyridyl-Azoles. Journal of Physical Chemistry B, 2006, 110, 8928-8934.	1.2	289
3	Conceptual density functional theory: status, prospects, issues. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	249
4	Recent advances in planar tetracoordinate carbon chemistry. Journal of Computational Chemistry, 2007, 28, 362-372.	1.5	211
5	A relationship between the static dipole polarizability, the global softness, and the fukui function. Journal of the American Chemical Society, 1990, 112, 1490-1492.	6.6	193
6	deMon2k. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 548-555.	6.2	189
7	Description of Electron Delocalization via the Analysis of Molecular Fields. Chemical Reviews, 2005, 105, 3812-3841.	23.0	160
8	Chemical reactivity in spin-polarized density functional theory. The Journal of Physical Chemistry, 1988, 92, 6470-6474.	2.9	146
9	Defining the Domain of Density Functionals: Charge-Transfer Complexes. Journal of the American Chemical Society, 1995, 117, 1141-1142.	6.6	133
10	Theoretical Analysis of the Smallest Carbon Cluster Containing a Planar Tetracoordinate Carbon. Journal of the American Chemical Society, 2004, 126, 16160-16169.	6.6	126
11	Planar Tetracoordinate Carbon in Extended Systems. Journal of the American Chemical Society, 2004, 126, 15309-15315.	6.6	126
12	Troubleshooting time-dependent density-functional theory for photochemical applications: Oxirane. Journal of Chemical Physics, 2007, 127, 164111.	1.2	124
13	The Implications of Symmetry of the External Potential on Bond Paths. Chemistry - A European Journal, 2008, 14, 10232-10234.	1.7	119
14	(C5M2-n)n- (M = Li, Na, K, and n = 0, 1, 2). A New Family of Molecules Containing Planar Tetracoordinate Carbons. Journal of the American Chemical Society, 2003, 125, 6026-6027.	6.6	96
15	Stereoelectronic Interpretation for the Anomalous 1H NMR Chemical Shifts and One-Bond C-H Coupling Constants (Perlin Effects) in 1,3-Dioxanes, 1,3-Oxathianes, and 1,3-Dithianes. Spectroscopic and Theoretical Observations. Journal of the American Chemical Society, 1994, 116, 5796-5804.	6.6	87
16	Molecular Quadrupole Moments for the Series of Fluoro- and Chlorobenzenes. The Journal of Physical Chemistry, 1996, 100, 6524-6530.	2.9	82
17	Determining and extending the domain of exchange and correlation functionals. International Journal of Quantum Chemistry, 1995, 56, 61-78.	1.0	80
18	Non-empirical improvement of PBE and its hybrid PBE0 for general description of molecular properties. Journal of Chemical Physics, 2012, 136, 104108.	1.2	78

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19	An efficient gridâ€based scheme to compute QTAIM atomic properties without explicit calculation of zeroâ€flux surfaces. Journal of Computational Chemistry, 2009, 30, 1082-1092.	1.5	73
20	Singletâ^'Triplet Gaps and Spin Potentials. Journal of Physical Chemistry A, 1998, 102, 3134-3140.	1.1	68
21	Density Functional Calculation of 1JC-H Coupling Constants in Cyclohexane and Diheterocyclohexanes. Repercussion of Stereoelectronic Effects on Coupling Constants. Journal of Physical Chemistry A, 1999, 103, 932-937.	1.1	68
22	Do Cooperative Protonâ^'Hydride Interactions Explain the Gasâ^'Solid Structural Difference of BH3NH3?. Journal of Physical Chemistry A, 2002, 106, 8491-8494.	1.1	68
23	Planar Tetracoordinate Carbons in Cyclic Hydrocarbons. Organic Letters, 2005, 7, 1509-1512.	2.4	68
24	Revisiting electroaccepting and electrodonating powers: proposals for local electrophilicity and local nucleophilicity descriptors. Physical Chemistry Chemical Physics, 2014, 16, 26832-26842.	1.3	68
25	Revisiting the definition of the electronic chemical potential, chemical hardness, and softness at finite temperatures. Journal of Chemical Physics, 2015, 143, 154103.	1.2	67
26	Nonlocal correlation functional involving the Laplacian of the density. Chemical Physics Letters, 1994, 230, 419-428.	1.2	65
27	Comparison of static polarizabilities of Cun, Nan, and Lin (nâ©½9) clusters. Journal of Chemical Physics, 2000, 113, 2199-2202.	1.2	64
28	Numerical self-consistent-field method to solve the Kohn-Sham equations in confined many-electron atoms. Physical Review E, 1998, 58, 3949-3954.	0.8	61
29	Local and linear chemical reactivity response functions at finite temperature in density functional theory. Journal of Chemical Physics, 2015, 143, 244117.	1.2	55
30	Local softness and chemical reactivity of maleimide: nucleophilic addition. Computational and Theoretical Chemistry, 1992, 277, 81-86.	1.5	54
31	Quadrupole interactions in pure non-dipolar fluorinated or methylated benzenes and their binary mixtures. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 2441-2443.	1.7	53
32	Spectroscopic and Electronic Structure Studies of Copper(II) Binding to His111 in the Human Prion Protein Fragment 106â^'115: Evaluating the Role of Protons and Methionine Residues. Inorganic Chemistry, 2011, 50, 1956-1972.	1.9	50
33	Parallelization of the deMon2k code. Journal of Computational Chemistry, 2006, 27, 483-490.	1.5	47
34	A new meta-GGA exchange functional based on an improved constraint-based GGA. Chemical Physics Letters, 2012, 543, 179-183.	1.2	44
35	Generalized gradient approximation exchange energy functional with correct asymptotic behavior of the corresponding potential. Journal of Chemical Physics, 2015, 142, 054105.	1.2	42
36	Chemically controlled self-assembly of [2]pseudorotaxanes based on 1,2-bis(benzimidazolium)ethane cations and 24-crown-8 macrocycles. Organic and Biomolecular Chemistry, 2007, 5, 2252-2256.	1.5	40

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37	Temperatureâ€dependent approach to chemical reactivity concepts in density functional theory. International Journal of Quantum Chemistry, 2019, 119, e25797.	1.0	40
38	Aluminum clusters. A comparison between all electron and model core potential calculations. Journal of Chemical Physics, 1994, 101, 10677-10685.	1.2	39
39	Rationalization of the anomalous 1H NMR chemical shifts in 1,3-diheterocyclohexanes. Computational and Theoretical Chemistry, 1997, 418, 231-241.	1.5	37
40	Donorâ^'Acceptor Heteroleptic Open Sandwiches. Inorganic Chemistry, 2006, 45, 1091-1095.	1.9	36
41	Variable Liebâ€“Oxford bound satisfaction in a generalized gradient exchange-correlation functional. Journal of Chemical Physics, 2009, 130, 244103.	1.2	36
42	Planar Tetracoordinate Carbons in Cyclic Semisaturated Hydrocarbons. Journal of Organic Chemistry, 2008, 73, 7037-7044.	1.7	35
43	Fukui function, electronegativity and hardness in the Kohn-Sham theory. , 1987, , 79-97.		33
44	Weak Intramolecular Protonâ^'Hydride and Protonâ^'Fluoride Interactions:Â Experimental (NMR, X-ray) and DFT Studies of the Bis(NBH3) and Bis(NBF3) Adducts of 1,3-Dimethyl-1,3-diazolidine. Journal of the American Chemical Society, 2001, 123, 9144-9152.	6.6	32
45	Copper coordination to the prion protein: Insights from theoretical studies. Coordination Chemistry Reviews, 2013, 257, 429-444.	9.5	32
46	Improved constraint satisfaction in a simple generalized gradient approximation exchange functional. Journal of Chemical Physics, 2012, 136, 144115.	1.2	31
47	The reduced density gradient in atoms. International Journal of Quantum Chemistry, 2012, 112, 3594-3598.	1.0	27
48	Going beyond the three-state ensemble model: the electronic chemical potential and Fukui function for the general case. Physical Chemistry Chemical Physics, 2017, 19, 11588-11602.	1.3	27
49	Thermodynamic Justification for the Parabolic Model for Reactivity Indicators with Respect to Electron Number and a Rigorous Definition for the Electrophilicity: The Essential Role Played by the Electronic Entropy. Journal of Chemical Theory and Computation, 2018, 14, 597-606.	2.3	27
50	Local chemical potential, local hardness, and dual descriptors in temperature dependent chemical reactivity theory. Physical Chemistry Chemical Physics, 2017, 19, 13687-13695.	1.3	26
51	Fukui function: Spinâ€density and chemical reactivity. Journal of Chemical Physics, 1986, 85, 2337-2338.	1.2	25
52	Stability of charged aluminum clusters. Physical Review B, 1994, 49, 17464-17467.	1.1	25
53	Structure and Energetics of Group 14 (IV-A) Halides:Â A Comparative Density Functional-Pseudopotential Study. Journal of Physical Chemistry A, 1999, 103, 5590-5601.	1.1	25
54	Atomic ionization radii using Janak's theorem. Chemical Physics Letters, 2000, 325, 29-32.	1.2	25

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55	Relationship between the electronic chemical potential and proton transfer barriers. Chemical Physics Letters, 1997, 269, 419-427.	1.2	24
56	Thermodynamic responses of electronic systems. Journal of Chemical Physics, 2017, 147, 094105.	1.2	24
57	Generalized Gradient Approximation Exchange Energy Functional with Near-Best Semilocal Performance. Journal of Chemical Theory and Computation, 2019, 15, 303-310.	2.3	24
58	Half-numerical evaluation of pseudopotential integrals. Journal of Computational Chemistry, 2006, 27, 1009-1019.	1.5	23
59	Local hardness equalization and the principle of maximum hardness. Journal of Chemical Physics, 2013, 138, 214103.	1.2	23
60	Thermodynamic hardness and the maximum hardness principle. Journal of Chemical Physics, 2017, 147, 074113.	1.2	22
61	Excitation energies from an auxiliary-function formulation of time-dependent density-functional response theory with charge conservation constraint. Computational and Theoretical Chemistry, 2006, 762, 179-191.	1.5	21
62	Structural Models for Cu(II) Bound to the Fragment 92â€“96 of the Human Prion Protein. Journal of Physical Chemistry B, 2013, 117, 789-799.	1.2	20
63	Global and Local Partitioning of the Charge Transferred in the Parrâ€“Pearson Model. Journal of Physical Chemistry A, 2017, 121, 4019-4029.	1.1	20
64	Reparameterization of a meta-generalized gradient approximation functional by combining TPSS exchange with Ï„1 correlation. Theoretical Chemistry Accounts, 2007, 118, 693-707.	0.5	19
65	Spectroscopic and Theoretical Study of Cu^I Binding to His111 in the Human Prion Protein Fragment 106â€“115. Inorganic Chemistry, 2016, 55, 2909-2922.	1.9	19
66	Tryptophan regulatesDrosophilazinc stores. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2117807119.	3.3	19
67	Static dipole and quadrupole polarizability of confined hydrogen atom withZ=N/3 (N=1-5). International Journal of Quantum Chemistry, 2002, 90, 491-496.	1.0	18
68	Study of the D?Sb (D = O, S) Transannular Interaction in Sb-Monohalogenated Dibenzostibocinesâ˜† An Experimental and Theoretical Study. European Journal of Inorganic Chemistry, 2003, 2003, 3554-3562.	1.0	18
69	Chemical reactivity in density functional theory: the N-differentiability problem. Computational and Theoretical Chemistry, 1990, 210, 29-38.	1.5	17
70	Donation and back-donation analyzed through a charge transfer model based on density functional theory. Journal of Molecular Modeling, 2017, 23, 207.	0.8	17
71	Chemical hardness: Temperature dependent definitions and reactivity principles. Journal of Chemical Physics, 2018, 149, 124110.	1.2	17
72	Nonlocal correlation functional involving the Laplacian of the density (Chem. Phys. Letters 230 (1994)) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.2	16

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73	Electronic chemical response indexes at finite temperature in the canonical ensemble. Journal of Chemical Physics, 2015, 143, 024112.	1.2	16
74	A PW91-like exchange with a simple analytical form. Chemical Physics Letters, 2016, 651, 268-273.	1.2	16
75	Role of N-terminal methionine residues in the redox activity of copper bound to alpha-synuclein. Journal of Biological Inorganic Chemistry, 2016, 21, 691-702.	1.1	16
76	Strongly convergent method to solve one-dimensional quantum problems. Physical Review E, 1996, 53, 1954-1963.	0.8	15
77	New Fukui, dual and hyper-dual kernels as bond reactivity descriptors. Physical Chemistry Chemical Physics, 2017, 19, 16095-16104.	1.3	15
78	Gradient-free exchange-correlation functional beyond the local-spin-density approximation. Physical Review A, 1994, 50, 3766-3774.	1.0	14
79	Role of Reaction Conditions in the Global and Local Two Parabolas Charge Transfer Model. Journal of Physical Chemistry A, 2018, 122, 1796-1806.	1.1	13
80	Radical grafting of carbon surfaces by oxidation of 5-nitroindole derived anions. Journal of Electroanalytical Chemistry, 2012, 670, 30-35.	1.9	11
81	Insights into the Oxygen-Based Ligand of the Low pH Component of the Cu2+-Amyloid-Î² Complex. Journal of Physical Chemistry B, 2014, 118, 10052-10064.	1.2	10
82	Global and local charge transfer in electron donor-acceptor complexes. Journal of Molecular Modeling, 2018, 24, 250.	0.8	10
83	Molecular Fragments in Density Functional Theory. Journal of Physical Chemistry A, 2006, 110, 4535-4537.	1.1	9
84	Chemical hardness and the discontinuity of the Kohn-Sham exchange-correlation potential. Journal of Chemical Physics, 2007, 126, 214105.	1.2	9
85	The reaction of [Fe3(CO)12] with HCCSiR3 (RÂ=ÂMe, Ph) and reactivity of [HFe3(CO)9(CCSiMe3)] with amines. Theoretical studies on NMR 1H and 13C chemical shifts and some advances in the theoretical determinations of pKa in cluster compounds. Journal of Organometallic Chemistry, 2014, 751, 420-429.	0.8	9
86	Generalized gradient approximations with local parameters. Physical Review B, 2020, 102, .	1.1	9
87	Study of organic reactions using chemical reactivity descriptors derived through a temperature-dependent approach. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	9
88	Achieving reliability of calculations for flat potential surfaces in density functional theory: The case of Al4 and Al4+1. International Journal of Quantum Chemistry, 1997, 63, 301-311.	1.0	8
89	Global hybrid exchange energy functional with correct asymptotic behavior of the corresponding potential. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	7
90	Theoretical approach to the conformational analyses of dithiazinane, thiadiazinane and triazinane, their N-borane adducts and Nâ€“H cations. Journal of Molecular Structure, 2016, 1113, 112-126.	1.8	7

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91	Spectroscopic properties of open shell diatomic molecules using Piris natural orbital functionals. Physical Chemistry Chemical Physics, 2021, 23, 2953-2963.	1.3	7
92	Behavior of the Chemical Potential of Neutral Atoms in the Limit of Large Nuclear Charge. Physical Review Letters, 1986, 56, 2606-2609.	2.9	6
93	Theoretical Study of the Thermal Dissociation Mechanism of AH4(A = Si, Ge, Sn, Pb). Journal of Physical Chemistry A, 2004, 108, 4909-4915.	1.1	6
94	Negative Electron Affinities and Derivative Discontinuity Contribution from a Generalized Gradient Approximation Exchange Functional. Journal of Physical Chemistry A, 2020, 124, 1334-1342.	1.1	6
95	On the oscillatory behavior of the chemical potential of neutral atoms. International Journal of Quantum Chemistry, 1988, 34, 329-335.	1.0	5
96	Reactivity of [H2Os3(CO)10] with six-membered heterocycles containing sulfur and/or nitrogen atoms. Cleavage of Câ€“S, Câ€“N and Câ€“H bonds to yield linked clusters with Sâ€“C, and Sâ€“Câ€“N bridging fragments. Journal of Organometallic Chemistry, 2014, 772-773, 248-257.	0.8	5
97	An Anionic Ring Locked into an Anionic Axle: A Metastable Rotaxane with Chemically Activated Electrostatic Stoppers. Chemistry - A European Journal, 2019, 25, 14042-14047.	1.7	5
98	Natural orbital functional for spin-polarized periodic systems. Journal of Physics Condensed Matter, 2019, 31, 165501.	0.7	5
99	Interatomic interactions in density functional theory. International Journal of Quantum Chemistry, 1986, 29, 937-948.	1.0	4
100	A new approach to second order corrections based on density functional theory. International Journal of Quantum Chemistry, 1988, 34, 71-76.	1.0	4
101	Comment on â€œ Eigenvalue spectrum of the independent-fermion kinetic-energy kernelâ€. Physical Review A, 1998, 58, 3358-3359.	1.0	4
102	Reduced density gradient as a novel approach for estimating QSAR descriptors, and its application to 1, 4-dihydropyridine derivatives with potential antihypertensive effects. Journal of Molecular Modeling, 2016, 22, 296.	0.8	4
103	Binding energies of atoms and ions: TheZâ^'1perturbation expansion and the Thomas-Fermi limit. Physical Review A, 1988, 38, 3264-3270.	1.0	3
104	The electroformation of a Ru + Ag surface alloy. Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, 1989, 261, 409-421.	0.3	3
105	Long-range exchange limit and dispersion in pure silica zeolites. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	3
106	Temperature-Dependent Approach to Electronic Charge Transfer. Journal of Physical Chemistry A, 2020, 124, 5465-5473.	1.1	3
107	Effective atomic charge distribution in molecules from multiple scattering calculations. Chemical Physics Letters, 1980, 73, 84-88.	1.2	2
108	Chapter 12 Theoretical design of electronically stabilized molecules containing planar tetracoordinate carbons. Theoretical and Computational Chemistry, 2007, , 251-267.	0.2	2

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109	Theoretical chemistry in Latin America. International Journal of Quantum Chemistry, 2019, 119, e25852.	1.0	2
110	Structural and electronic analysis of the octarepeat region of prion protein with four Cu2+ by polarizable MD and QM/MM simulations. Physical Chemistry Chemical Physics, 2021, 23, 21568-21578.	1.3	2
111	The square-planar structure of bis[N-(i-propyl)-3-oxy-2-naphthaldiminato]copper(II). Journal of Coordination Chemistry, 2014, 67, 2405-2414.	0.8	1
112	Temperature effects in static and dynamic polarizabilities from distinct generalized gradient approximation exchange-correlation functionals. Chemical Physics Letters, 2016, 664, 77-82.	1.2	1
113	An ab-initio electronic structure study of the chemisorption of small molecules in aluminum cluster ions. Scripta Materialia, 1993, 2, 157-162.	0.5	0
114	Reply to â€œComment on â€˜Strongly convergent method to solve one-dimensional quantum problemsâ€™ â€• Physical Review E, 1997, 56, 1283-1284.	0.8	0
115	Theoretical Study of the Thermal Dissociation Mechanism of AH4 (A: Si, Ge, Sn, Pb).. ChemInform, 2004, 35, no.	0.1	0
116	Description of Electron Delocalization via the Analysis of Molecular Fields. ChemInform, 2006, 37, no.	0.1	0
117	An Exchange-Correlation Potential With Built in Discontinuity and Correct Long Range Behavior. AIP Conference Proceedings, 2008, , .	0.3	0
118	Electronic structure of dichloro-bridged ruthenium(II) dimers. International Journal of Quantum Chemistry, 2009, 18, 191-200.	1.0	0
119	Reversible stereoisomerâ€specific Cotton effect of the ligand field transitions at a Cu(II) binding site of the prion protein. European Journal of Inorganic Chemistry, 0, , .	1.0	0
120	Introduction to celebrating recent chemical science in Mexico. RSC Advances, 2021, 11, 891-892.	1.7	0
121	Structural Phase Transitions in Cesium Halides. , 1991, , 293-306.		0