Miquel Duran

List of Publications by Year
in descending order

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125 papers	8,392 citations	53794 45 h-index	45317 90 g-index
127 all docs	127 docs citations	127 times ranked	6098 citing authors

#	Article	IF	Citations
1	How does basis set superposition error change the potential surfaces for hydrogenâ€bonded dimers?. Journal of Chemical Physics, 1996, 105, 11024-11031.	3.0	1,882
2	Theoretical Evaluation of Electron Delocalization in Aromatic Molecules by Means of Atoms in Molecules (AIM) and Electron Localization Function (ELF) Topological Approaches. Chemical Reviews, 2005, 105, 3911-3947.	47.7	661
3	The Delocalization Index as an Electronic Aromaticity Criterion: Application to a Series of Planar Polycyclic Aromatic Hydrocarbons. Chemistry - A European Journal, 2003, 9, 400-406.	3.3	396
4	The aromatic fluctuation index (FLU): A new aromaticity index based on electron delocalization. Journal of Chemical Physics, 2005, 122, 014109.	3.0	396
5	Electron sharing indexes at the correlated level. Application to aromaticity calculations. Faraday Discussions, 2007, 135, 325-345.	3.2	203
6	The calculation of electron localization and delocalization indices at the Hartree-Fock, density functional and post-Hartree-Fock levels of theory. Theoretical Chemistry Accounts, 2002, 107, 362-371.	1.4	187
7	Electron-pairing analysis from localization and delocalization indices in the framework of the atoms-in-molecules theory. Theoretical Chemistry Accounts, 2002, 108, 214-224.	1.4	175
8	Comparison of the AIM Delocalization Index and the Mayer and Fuzzy Atom Bond Orders. Journal of Physical Chemistry A, 2005, 109, 9904-9910.	2.5	169
9	Electron localization function at the correlated level. Journal of Chemical Physics, 2006, 125, 024301.	3.0	135
10	Effect of Basis Set Superposition Error on the Water Dimer Surface Calculated at Hartreeâ^'Fock, MÃ¸llerâ^'Plesset, and Density Functional Theory Levels. Journal of Physical Chemistry A, 1999, 103, 1640-1643.	2.5	128
11	An Insight into the Local Aromaticities of Polycyclic Aromatic Hydrocarbons and Fullerenes. Chemistry - A European Journal, 2003, 9, 1113-1122.	3.3	125
12	Analysis of solvent effects on the Menshutkin reaction. Journal of the American Chemical Society, 1991, 113, 2873-2879.	13.7	123
13	Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. Journal of Chemical Theory and Computation, 2010, 6, 2736-2742.	5.3	115
14	On the Validity of the Maximum Hardness and Minimum Polarizability Principles for Nontotally Symmetric Vibrations. Journal of the American Chemical Society, 2001, 123, 7951-7952.	13.7	112
15	Fine-Tuning the Electronic Properties of Highly Stable Organometallic CuIII Complexes Containing Monoanionic Macrocyclic Ligands. Chemistry - A European Journal, 2005, 11, 5146-5156.	3.3	106
16	Basis set and electron correlation effects on ab initio electronic and vibrational nonlinear optical properties of conjugated organic molecules. Journal of Chemical Physics, 2003, 118, 711-718.	3.0	105
17	Molecular Structure and Bonding of Copper Cluster Monocarbonyls CunCO (n= 1â^'9). Journal of Physical Chemistry B, 2006, 110, 6526-6536.	2.6	97
18	On the effect of the BSSE on intermolecular potential energy surfaces. Comparison ofa priori anda posteriori BSSE correction schemes. Journal of Computational Chemistry, 2001, 22, 765-786.	3.3	93

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19	Mechanism of the Addition Reaction of Alkyl Azides to [60]Fullerene and the Subsequent N2Extrusion to Form Monoimino-[60]fullerenes. Journal of Organic Chemistry, 2001, 66, 433-442.	3.2	91
20	Finite field treatment of vibrational polarizabilities and hyperpolarizabilities: On the role of the Eckart conditions, their implementation, and their use in characterizing key vibrations. Journal of Chemical Physics, 1999, 111, 875-884.	3.0	82
21	Molecular Structure and Bond Characterization of the Fischer-Type Chromiumâ˜'Carbene Complexes (CO)5CrC(X)R (X = H, OH, OCH3, NH2, NHCH3 and R = H, CH3, CHCH2, Ph, Câ‹®CH). Organometallics, 2002, 21, 4182-4191.	2.3	80
22	Theoretical Evaluation of Solvent Effects on the Conformational and Tautomeric Equilibria of 2-(2â€˜-Hydroxyphenyl)benzimidazole and on Its Absorption and Fluorescence Spectra. Journal of Physical Chemistry A, 1999, 103, 4525-4532.	2.5	79
23	Are the maximum hardness and minimum polarizability principles always obeyed in nontotally symmetric vibrations?. Journal of Chemical Physics, 2002, 117, 10561-10570.	3.0	77
24	Aromaticity Measures from Fuzzy-Atom Bond Orders (FBO). The Aromatic Fluctuation (FLU) and the para-Delocalization (PDI) Indexes. Journal of Physical Chemistry A, 2006, 110, 5108-5113.	2.5	76
25	Determination of vibrational polarizabilities and hyperpolarizabilities using field-induced coordinates. Journal of Chemical Physics, 2000, 113, 5203.	3.0	72
26	Intramolecular basis set superposition error effects on the planarity of benzene and other aromatic molecules: A solution to the problem. Journal of Chemical Physics, 2008, 128, 144108.	3.0	72
27	Ab initio study of the hydration of carbon dioxide by carbonic anhydrase. A comparison between the Lipscomb and Lindskog mechanisms. Journal of the American Chemical Society, 1992, 114, 869-877.	13.7	70
28	Molecular electric properties and nuclear and vibrational relaxation. Molecular Physics, 1993, 80, 625-633.	1.7	67
29	A systematic and feasible method for computing nuclear contributions to electrical properties of polyatomic molecules. Journal of Chemical Physics, 1997, 107, 1501-1512.	3.0	67
30	Theoretical Study of Dielsâ˜'Alder Cycloadditions of Butadiene to C70. An Insight into the Chemical Reactivity of C70as Compared to C60. The Journal of Physical Chemistry, 1996, 100, 7449-7454.	2.9	64
31	Nuclear relaxation contribution to static and dynamic (infinite frequency approximation) nonlinear optical properties by means of electrical property expansions: Application to HF, CH4, CF4, and SF6. Journal of Chemical Physics, 1998, 108, 4123-4130.	3.0	63
32	Copper(II) Hexaaza Macrocyclic Binuclear Complexes Obtained from the Reaction of Their Copper(I) Derivates and Molecular Dioxygen. Inorganic Chemistry, 2006, 45, 3569-3581.	4.0	61
33	Basis set and electron correlation effects on initial convergence for vibrational nonlinear optical properties of conjugated organic molecules. Journal of Chemical Physics, 2004, 120, 6346-6355.	3.0	60
34	An analysis of the changes in aromaticity and planarity along the reaction path of the simplest Dielsâ€“Alder reaction. Exploring the validity of different indicators of aromaticity. Computational and Theoretical Chemistry, 2005, 727, 165-171.	1.5	59
35	Aromaticity and electronic delocalization in all-metal clusters with single, double, and triple aromatic character. Theoretical Chemistry Accounts, 2011, 128, 419-431.	1.4	57
36	Use of ab Initio Quantum Molecular Similarities as an Interpretative Tool for the Study of Chemical Reactions. Journal of the American Chemical Society, 1994, 116, 5909-5915.	13.7	54

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37	A comparative analysis by means of quantum molecular similarity measures of density distributions derived from conventional ab initio and density functional methods. Journal of Chemical Physics, 1996, 104, 636-647.	3.0	54
38	Anharmonicity contributions to the vibrational second hyperpolarizability of conjugated oligomers. Journal of Chemical Physics, 2000, 112, 1011-1019.	3.0	54
39	Analysis of the effect of changing the a0 parameter of the Becke3-LYP hybrid functional on the transition state geometries and energy barriers in a series of prototypical reactions. Physical Chemistry Chemical Physics, 2002, 4, 722-731.	2.8	51
40	Molecular Size and Pyramidalization: Two Keys for Understanding the Reactivity of Fullerenes. The Journal of Physical Chemistry, 1995, 99, 10752-10758.	2.9	50
41	An AM1 study of the reactivity of buckminsterfullerene (C60) in a Diels-Alder model reaction. Chemical Physics Letters, 1994, 231, 325-330.	2.6	49
42	Intermolecular bond lengths: extrapolation to the basis set limit on uncorrected and BSSE-corrected potential energy hypersurfaces. Journal of Computational Chemistry, 2001, 22, 196-207.	3.3	49
43	On the calculation ofab initioquantum molecular similarities for large systems: Fitting the electron density. Journal of Computational Chemistry, 1994, 15, 1113-1120.	3.3	46
44	Counterpoise Corrected Ion/Molecule Complexes Using Two or Three Fragments. Journal of Physical Chemistry A, 2002, 106, 6883-6889.	2.5	46
45	Electron Fluctuation in Pericyclic and Pseudopericyclic Reactions. ChemPhysChem, 2006, 7, 111-113.	2.1	45
46	Initial convergence of the perturbation series expansion for vibrational nonlinear optical properties. Journal of Chemical Physics, 2002, 116, 5363-5373.	3.0	43
47	Field-induced coordinates for the determination of dynamic vibrational nonlinear optical properties. Journal of Chemical Physics, 2001, 115, 4473-4483.	3.0	41
48	New Ru Complexes Containing the N-Tridentate bpea and Phosphine Ligands:Â Consequences of Meridional vs Facial Geometry. Inorganic Chemistry, 2006, 45, 10520-10529.	4.0	41
49	Aromaticity Determines the Relative Stability of Kinked vs. Straight Topologies in Polycyclic Aromatic Hydrocarbons. Frontiers in Chemistry, 2018, 6, 561.	3.6	41
50	Theoretical Study of the Regioselectivity of Successive 1,3-Butadiene Dielsâ^'Alder Cycloadditions to C60. Journal of the American Chemical Society, 1996, 118, 8920-8924.	13.7	37
51	Weighing Different Mechanistic Proposals for the DÃ¶tz Reaction:Â A Density Functional Study. Journal of the American Chemical Society, 1999, 121, 1309-1316.	13.7	37
52	Density functional energy decomposition into one- and two-atom contributions. Journal of Chemical Physics, 2005, 122, 244110.	3.0	36
53	Density Functional Study on the Preactivation Scenario of the DÃ¶tz Reaction:â€‰ Carbon Monoxide Dissociation versus Alkyne Addition as the First Reaction Step. Organometallics, 1998, 17, 1492-1501.	2.3	34
54	New Insights in Chemical Reactivity by Means of Electron Pairing Analysis. Journal of Physical Chemistry A, 2001, 105, 2052-2063.	2.5	34

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55	Effects of Solvation on the Pairing of Electrons in a Series of Simple Molecules and in the Menshutkin Reaction. Journal of Physical Chemistry A, 2001, 105, 6249-6257.	2.5	32
56	The hardness profile as a tool to detect spurious stationary points in the potential energy surface. Journal of Chemical Physics, 2004, 120, 10914-10924.	3.0	32
57	Dihydrogen Bonding: Donorâ€“Acceptor Bonding (AHâ‹…â‹…â‹…HX) versus the H₂ Molecule (Aï£¿H₂ï£¿X). Chemistry - A European Journal, 2009, 15, 5814-5822.	3.3	32
58	Anion binding and pentacoordination in zinc(II) complexes. Inorganic Chemistry, 1991, 30, 2523-2527.	4.0	31
59	The use of ab initio quantum molecular self-similarity measures to analyze electronic charge density distributions. International Journal of Quantum Chemistry, 1998, 58, 361-372.	2.0	31
60	An assessment of a simple hardness kernel approximation for the calculation of the global hardness in a series of Lewis acids and bases. Computational and Theoretical Chemistry, 2005, 727, 139-148.	1.5	31
61	Atropisomeric Discrimination in New RuII Complexes Containing theC2-Symmetric Didentate Chiral Phenyl-1,2-bisoxazolinic Ligand. Chemistry - A European Journal, 2006, 12, 2798-2807.	3.3	30
62	Is coronene better described by <scp>C</scp>lar's aromatic Ï€â€sextet model or by the AdNDP representation?. Journal of Computational Chemistry, 2017, 38, 1606-1611.	3.3	30
63	Global Hardness Evaluation Using Simplified Models for the Hardness Kernel. Journal of Physical Chemistry A, 2002, 106, 4632-4638.	2.5	29
64	Electron Density Topological Properties Are Useful To Assess the Difference between Hydrogen and Dihydrogen Complexes. Journal of Physical Chemistry A, 2007, 111, 4506-4512.	2.5	29
65	The relevance of the Laplacian of intracule and extracule density distributions for analyzing electronâ€“electron interactions in molecules. Journal of Chemical Physics, 1997, 107, 3576-3583.	3.0	28
66	Metal Cluster Electrides: A New Type of Molecular Electride with Delocalised Polyattractor Character. Chemistry - A European Journal, 2018, 24, 9853-9859.	3.3	28
67	Tuning the Strength of the Resonance-Assisted Hydrogen Bond in o-Hydroxybenzaldehyde by Substitution in the Aromatic Ring¹. Journal of Physical Chemistry A, 2018, 122, 2279-2287.	2.5	28
68	An assessment of density functional theory on evaluating activation barriers for small organic gas-phase rearrangement reactions. Computational and Theoretical Chemistry, 1996, 362, 163-173.	1.5	27
69	Generalizing the Breakdown of the Maximum Hardness and Minimum Polarizabilities Principles for Nontotally Symmetric Vibrations to Non-Ï€-Conjugated Organic Molecules. Journal of Physical Chemistry A, 2005, 109, 615-621.	2.5	26
70	Ab Initio Quantum Molecular Similarity Measures on Metal-Substituted Carbonic Anhydrase (MIICA, M) Tj ETQq0 0 0 rgBT /Overlock 10 T 1047-1053.	2.8	25
71	The effect of counterpoise correction and relaxation energy term to the internal rotation barriers: Application to the BF3â‹¯NH3 and C2H4â‹¯SO2 dimers. Journal of Chemical Physics, 1999, 111, 4460-4465.	3.0	25
72	The use of ab initio quantum molecular selfâ€similarity measures to analyze electronic charge density distributions. International Journal of Quantum Chemistry, 1996, 58, 361-372.	2.0	25

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73	Systematic study of the static electrical properties of the CO molecule: Influence of the basis set size and correlation energy. Journal of Chemical Physics, 1995, 102, 7573-7583.	3.0	24
74	Intramolecular proton transfer in the ground and the two lowest-lying singlet excited states of 1-amino-3-propenal and related species. Chemical Physics, 1998, 234, 1-19.	1.9	24
75	Effect of basis set superposition error on the electron density of molecular complexes. Journal of Chemical Physics, 2000, 112, 10106-10115.	3.0	24
76	Counterpoise-corrected potential energy surfaces for dihydrogen bonded systems. Chemical Physics Letters, 2004, 386, 373-376.	2.6	24
77	Intramolecular Basis Set Superposition Error Effects on the Planarity of DNA and RNA Nucleobases. Journal of Chemical Theory and Computation, 2009, 5, 2574-2581.	5.3	23
78	Substituent effects on the intramolecular proton transfer in the ground and lowest-lying singlet excited states of salicylaldimine. Chemical Physics, 2000, 260, 53-64.	1.9	22
79	Nonadiabatic and Bornâ€“Oppenheimer calculations of the polarizabilites of LiH and LiD. Computational and Theoretical Chemistry, 2003, 633, 113-122.	1.5	22
80	Relations among several nuclear and electronic density functional reactivity indexes. Journal of Chemical Physics, 2003, 119, 9393-9400.	3.0	22
81	MHâ‹…sHX Dihydrogen Bond with Mâ‰¡Li, Na and Xâ‰¡F, Cl, Br: A CP-Corrected PES Calculation and an AIM Analysis. Structural Chemistry, 2005, 16, 257-263.	2.0	22
82	Parametrization of the Becke3-LYP hybrid functional for a series of small molecules using quantum molecular similarity techniques. Journal of Computational Chemistry, 2001, 22, 1666-1678.	3.3	21
83	A Novel Exploration of the Hartreeâ€“Fock Homolytic Bond Dissociation Problem in the Hydrogen Molecule by Means of Electron Localization Measures. Journal of Chemical Education, 2006, 83, 1243.	2.3	19
84	Electron pairing analysis of the Fischer-type chromiumâ€“carbene complexes (CO)5Crî…C(X)R (X=H, OH,) Tj ETQq0 0 0 rgBT /Overlock	1.9	18
85	Evaluation of the Analogy between Exceptions to the Generalized Maximum Hardness Principle for Non-Totally-Symmetric Vibrations and the Pseudo-Jahnâ€“Teller Effect. Journal of Physical Chemistry A, 2003, 107, 7337-7339.	2.5	18
86	Vibrational Stark effect and vibrational static electric properties of N2O. International Journal of Quantum Chemistry, 1994, 52, 9-15.	2.0	17
87	Comment on the â€œNature of Bonding in the Thermal Cyclization of (Z)-1,2,4,6-Heptatetraene and Its Heterosubstituted Analoguesâ€• Journal of Physical Chemistry B, 2005, 109, 7591-7593.	2.6	17
88	From glycerol to chlorohydrin esters using a solvent-free system. Microwave irradiation versus conventional heating. Tetrahedron, 2009, 65, 10370-10376.	1.9	17
89	Proton transfer in the water dimer catalyzed by doubly charged cations (Zn+2, Be+2, and Mg+2). Theoretica Chimica Acta, 1992, 81, 303-318.	0.8	16
90	Buckycatcher. A New Opportunity for Charge-Transfer Mediation?. Journal of Physical Chemistry C, 2008, 112, 1672-1678.	3.1	16

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91	The [2+1] Cycloaddition of Singlet Oxycarbonylnitrenes to C 60. Journal of Molecular Modeling, 2000, 6, 205-212.	1.8	14
92	The DÃ¶tz Reaction: A Chromium Fischer Carbene-Mediated Benzannulation Reaction. Catalysis By Metal Complexes, 2002, , 269-287.	0.6	13
93	Tuning the Strength of the Resonance-Assisted Hydrogen Bond in Acenes and Phenacenes with Two o-Hydroxyaldehyde Groupsâ€"The Importance of Topology. Journal of Organic Chemistry, 2019, 84, 15538-15548.	3.2	13
94	Octahedral aromaticity in ^{2S+1}A_{1g} X₆^q clusters (X =) Tj ETQq0 0 0 rgBT /Overlock	2.8	12
95	Second-order quantum similarity measures from intracule and extracule densities. Theoretical Chemistry Accounts, 1998, 99, 44-52.	1.4	11
96	Theoretical characterization of intramolecular proton transfer in the ground and the lowest-lying triplet excited states of 1-amino-3-propenal: a methodological comparison. Journal of Computational Chemistry, 2000, 21, 257-269.	3.3	11
97	Atomic transferability within the exchange-correlation density. Journal of Computational Chemistry, 2000, 21, 1361-1374.	3.3	11
98	Interpretation of Molecular Intracule and Extracule Density Distributions in Terms of Valence Bond Structures:â€‰ Two-Electron Systems and Processes. Journal of Physical Chemistry A, 2000, 104, 8445-8454.	2.5	11
99	Density functional theory study of the structures and stabilities of CuO and CuO3. International Journal of Quantum Chemistry, 2001, 81, 162-168.	2.0	11
100	Ab initio calculations on the [Rh(PH3)3Cl] system. Influence of the basis set on the structural and reactivity trends of transition-metal complexes. Journal of the Chemical Society, Faraday Transactions, 1992, 88, 1111-1117.	1.7	9
101	Quantum Chemical Study of the Reactivity of C60HR and C60(CHR) Derivatives. Journal of Organic Chemistry, 2004, 69, 2374-2380.	3.2	9
102	Excess charge delocalization in organic and biological molecules: some theoretical notions. Theoretical Chemistry Accounts, 2009, 123, 29-40.	1.4	9
103	Molecular hydrogen complex vs dihydride in ML4 + H2 systems. Influence of the ML4 fragment geometry. Inorganic Chemistry, 1989, 28, 2984-2988.	4.0	8
104	A chemical Hamiltonian approach study of the basis set superposition error changes on electron densities and one- and two-center energy components. Journal of Chemical Physics, 2002, 116, 6443-6457.	3.0	8
105	Charge-density concentration and electron-electron coalescence density in atoms and molecules. Physical Review A, 2000, 62, .	2.5	7
106	Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. Journal of Chemical Theory and Computation, 2011, 7, 1231-1231.	5.3	7
107	Analytic energy third derivatives for pairedâ€excited multiconfiguration selfâ€consistentâ€field wave functions. Journal of Chemical Physics, 1989, 90, 334-345.	3.0	6
108	AM1 study of a substituent transfer by means of a Dielsâ€“Alder and retro-Dielsâ€“Alder tandem reaction. Journal of the Chemical Society Perkin Transactions II, 1995, , 605-608.	0.9	5

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109	Theoretical study of the second-order vibrational Stark effect. Molecular Physics, 2000, 98, 513-520.	1.7	4
110	Basis set effects on the energy and hardness profiles of the hydrogen fluoride dimer. Journal of Chemical Sciences, 2005, 117, 549-554.	1.5	4
111	BSSE-free hardness profiles of hydrogen bond exchange in the hydrogen fluoride dimer. International Journal of Quantum Chemistry, 2006, 106, 2910-2919.	2.0	4
112	A quantum molecular similarity analysis of changes in molecular electron density caused by basis set flotation and electric field application. Journal of Chemical Physics, 1997, 107, 1529-1535.	3.0	3
113	Valence-bond calculations on ZNO and HGO using integrals computed through the semiempiricalAM1 method. International Journal of Quantum Chemistry, 1992, 44, 887-895.	2.0	2
114	Chapter 3 The breakdown of the maximum hardness and minimum polarizability principles for nontotally symmetric vibrations. Theoretical and Computational Chemistry, 2007, , 31-45.	0.4	2
115	Theoretical Study of the Catalyzed Hydration of CO2 by Carbonic Anhydrase: A Brief Overview.. , 1992, , 263-298.		2
116	Optimizing hybrid density functionals by means of quantum molecular similarity techniques. Advances in Molecular Similarity, 1999, , 187-203.	0.5	2
117	Ab initio. Theoretica Chimica Acta, 1995, 91, 333.	0.8	2
118	Intrinsic reaction coordinate of perturbed potential energy surfaces: Construction of perturbed energy profiles. International Journal of Quantum Chemistry, 1993, 47, 307-317.	2.0	1
119	Ab initio study of the HCO 3 ? /H2O exchange in the (NH3)3 ZnII(HCO 3 ?) complex. Theoretica Chimica Acta, 1995, 91, 333-351.	0.8	1
120	Comparison of quantum similarity measures derived from one-electron, intracule, and extracule densities. Advances in Molecular Similarity, 1999, , 215-243.	0.5	1
121	An Insight into the Local Aromaticities of Polycyclic Aromatic Hydrocarbons and Fullerenes.. ChemInform, 2003, 34, no.	0.0	0
122	Quantum Chemical Study of the Reactivity of C60HR and C60(CHR) Derivatives.. ChemInform, 2004, 35, no.	0.0	0
123	Theoretical Evaluation of Electron Delocalization in Aromatic Molecules by Means of Atoms in Molecules (AIM) and Electron Localization Functional (ELF) Topological Approaches. ChemInform, 2006, 37, no.	0.0	0
124	Quantitative assessment of the effect of basis set superposition error on the electron density of molecular complexes by means of quantum molecular similarity measures. International Journal of Quantum Chemistry, 2009, 109, 2572-2580.	2.0	0
125	GIRONAâ€™S CHEMICAL ITINERARY: 14 YEARS AND A PANDEMIC. INTED Proceedings, 2022, , .	0.0	0