Miquel Duran

List of Publications by Year in descending order

125 papers	8,392 citations	61687 45 h-index	51423 90 g-index
127 all docs	127 docs citations	127 times ranked	6788 citing authors

#	Article	IF	Citations
1	GIRONAâ€™S CHEMICAL ITINERARY: 14 YEARS AND A PANDEMIC. INTED Proceedings, 2022, , .	0.0	0
2	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.	1.7	13
3	Metal Cluster Electrides: A New Type of Molecular Electride with Delocalised Polyattractor Character. Chemistry - A European Journal, 2018, 24, 9853-9859.	1.7	28
4	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.	1.1	28
5	Aromaticity Determines the Relative Stability of Kinked vs. Straight Topologies in Polycyclic Aromatic Hydrocarbons. Frontiers in Chemistry, 2018, 6, 561.	1.8	41
6	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.	1.5	30
7	Octahedral aromaticity in ^{2S+1}A_{1g} X₆^q clusters (X =) Tj ETQq1 1 0.784314 rgBT	1.3	12
8	Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. Journal of Chemical Theory and Computation, 2011, 7, 1231-1231.	2.3	7
9	Aromaticity and electronic delocalization in all-metal clusters with single, double, and triple aromatic character. Theoretical Chemistry Accounts, 2011, 128, 419-431.	0.5	57
10	Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. Journal of Chemical Theory and Computation, 2010, 6, 2736-2742.	2.3	115
11	Dihydrogen Bonding: Donorâ€"Acceptor Bonding (AHâ‹…â‹…â‹…HX) versus the H₂ Molecule (Aï£¿H₂ï£¿X). Chemistry - A European Journal, 2009, 15, 5814-5822.	1.7	32
12	Excess charge delocalization in organic and biological molecules: some theoretical notions. Theoretical Chemistry Accounts, 2009, 123, 29-40.	0.5	9
13	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.	1.0	0
14	From glycerol to chlorohydrin esters using a solvent-free system. Microwave irradiation versus conventional heating. Tetrahedron, 2009, 65, 10370-10376.	1.0	17
15	Intramolecular Basis Set Superposition Error Effects on the Planarity of DNA and RNA Nucleobases. Journal of Chemical Theory and Computation, 2009, 5, 2574-2581.	2.3	23
16	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.	1.2	72
17	Buckycatcher. A New Opportunity for Charge-Transfer Mediation?. Journal of Physical Chemistry C, 2008, 112, 1672-1678.	1.5	16
18	Chapter 3 The breakdown of the maximum hardness and minimum polarizability principles for nontotally symmetric vibrations. Theoretical and Computational Chemistry, 2007, , 31-45.	0.2	2

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19	Electron sharing indexes at the correlated level. Application to aromaticity calculations. Faraday Discussions, 2007, 135, 325-345.	1.6	203
20	Electron Density Topological Properties Are Useful To Assess the Difference between Hydrogen and Dihydrogen Complexes. Journal of Physical Chemistry A, 2007, 111, 4506-4512.	1.1	29
21	Copper(II) Hexaaza Macrocyclic Binuclear Complexes Obtained from the Reaction of Their Copper(I) Derivates and Molecular Dioxygen. Inorganic Chemistry, 2006, 45, 3569-3581.	1.9	61
22	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.	1.1	76
23	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.	1.1	19
24	New Ru Complexes Containing the N-Tridentate bpea and Phosphine Ligands:Â Consequences of Meridional vs Facial Geometry. Inorganic Chemistry, 2006, 45, 10520-10529.	1.9	41
25	Electron localization function at the correlated level. Journal of Chemical Physics, 2006, 125, 024301.	1.2	135
26	Molecular Structure and Bonding of Copper Cluster Monocarbonyls CunCO (n= 1â^'9). Journal of Physical Chemistry B, 2006, 110, 6526-6536.	1.2	97
27	BSSE-free hardness profiles of hydrogen bond exchange in the hydrogen fluoride dimer. International Journal of Quantum Chemistry, 2006, 106, 2910-2919.	1.0	4
28	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.	0.1	0
29	Atropisomeric Discrimination in New RuII Complexes Containing theC2-Symmetric Didentate Chiral Phenyl-1,2-bisoxazolinic Ligand. Chemistry - A European Journal, 2006, 12, 2798-2807.	1.7	30
30	Electron Fluctuation in Pericyclic and Pseudopericyclic Reactions. ChemPhysChem, 2006, 7, 111-113.	1.0	45
31	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
32	Fine-Tuning the Electronic Properties of Highly Stable Organometallic CuIII Complexes Containing Monoanionic Macrocyclic Ligands. Chemistry - A European Journal, 2005, 11, 5146-5156.	1.7	106
33	Basis set effects on the energy and hardness profiles of the hydrogen fluoride dimer. Journal of Chemical Sciences, 2005, 117, 549-554.	0.7	4
34	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.	1.0	22
35	Density functional energy decomposition into one- and two-atom contributions. Journal of Chemical Physics, 2005, 122, 244110.	1.2	36
36	The aromatic fluctuation index (FLU): A new aromaticity index based on electron delocalization. Journal of Chemical Physics, 2005, 122, 014109.	1.2	396

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37	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
38	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.	23.0	661
39	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.	1.1	26
40	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.	1.2	17
41	Comparison of the AIM Delocalization Index and the Mayer and Fuzzy Atom Bond Orders. Journal of Physical Chemistry A, 2005, 109, 9904-9910.	1.1	169
42	The hardness profile as a tool to detect spurious stationary points in the potential energy surface. Journal of Chemical Physics, 2004, 120, 10914-10924.	1.2	32
43	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.	1.2	60
44	Quantum Chemical Study of the Reactivity of C60HR and C60(CHR) Derivatives.. ChemInform, 2004, 35, no.	0.1	0
45	Counterpoise-corrected potential energy surfaces for dihydrogen bonded systems. Chemical Physics Letters, 2004, 386, 373-376.	1.2	24
46	Quantum Chemical Study of the Reactivity of C60HR and C60(CHR) Derivatives. Journal of Organic Chemistry, 2004, 69, 2374-2380.	1.7	9
47	An Insight into the Local Aromaticities of Polycyclic Aromatic Hydrocarbons and Fullerenes.. ChemInform, 2003, 34, no.	0.1	0
48	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.	1.7	396
49	An Insight into the Local Aromaticities of Polycyclic Aromatic Hydrocarbons and Fullerenes. Chemistry - A European Journal, 2003, 9, 1113-1122.	1.7	125
50	Electron pairing analysis of the Fischer-type chromiumâ€“carbene complexes (CO)5Crî...C(X)R (X=H, OH,) Tj ETQq0 0 0 rgBT /Overlock	0.9	18
51	Nonadiabatic and Bornâ€“Oppenheimer calculations of the polarizabilites of LiH and LiD. Computational and Theoretical Chemistry, 2003, 633, 113-122.	1.5	22
52	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.	1.1	18
53	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.	1.2	105
54	Relations among several nuclear and electronic density functional reactivity indexes. Journal of Chemical Physics, 2003, 119, 9393-9400.	1.2	22

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55	Are the maximum hardness and minimum polarizability principles always obeyed in nontotally symmetric vibrations?. Journal of Chemical Physics, 2002, 117, 10561-10570.	1.2	77
56	The DÃ¶tz Reaction: A Chromium Fischer Carbene-Mediated Benzannulation Reaction. Catalysis By Metal Complexes, 2002, , 269-287.	0.6	13
57	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.	1.1	80
58	Counterpoise Corrected Ion/Molecule Complexes Using Two or Three Fragments. Journal of Physical Chemistry A, 2002, 106, 6883-6889.	1.1	46
59	Global Hardness Evaluation Using Simplified Models for the Hardness Kernel. Journal of Physical Chemistry A, 2002, 106, 4632-4638.	1.1	29
60	Initial convergence of the perturbation series expansion for vibrational nonlinear optical properties. Journal of Chemical Physics, 2002, 116, 5363-5373.	1.2	43
61	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.	1.3	51
62	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.	1.2	8
63	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.	0.5	187
64	Electron-pairing analysis from localization and delocalization indices in the framework of the atoms-in-molecules theory. Theoretical Chemistry Accounts, 2002, 108, 214-224.	0.5	175
65	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.	6.6	112
66	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.	1.7	91
67	New Insights in Chemical Reactivity by Means of Electron Pairing Analysis. Journal of Physical Chemistry A, 2001, 105, 2052-2063.	1.1	34
68	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.	1.1	32
69	Density functional theory study of the structures and stabilities of CuO and CuO3. International Journal of Quantum Chemistry, 2001, 81, 162-168.	1.0	11
70	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.	1.5	49
71	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.	1.5	93
72	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.	1.5	21

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73	Field-induced coordinates for the determination of dynamic vibrational nonlinear optical properties. Journal of Chemical Physics, 2001, 115, 4473-4483.	1.2	41
74	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.	1.5	11
75	Atomic transferability within the exchange-correlation density. Journal of Computational Chemistry, 2000, 21, 1361-1374.	1.5	11
76	Substituent effects on the intramolecular proton transfer in the ground and lowest-lying singlet excited states of salicylaldimine. Chemical Physics, 2000, 260, 53-64.	0.9	22
77	The [2+1] Cycloaddition of Singlet Oxycarbonylnitrenes to C 60. Journal of Molecular Modeling, 2000, 6, 205-212.	0.8	14
78	Charge-density concentration and electron-electron coalescence density in atoms and molecules. Physical Review A, 2000, 62, .	1.0	7
79	Determination of vibrational polarizabilities and hyperpolarizabilities using field-induced coordinates. Journal of Chemical Physics, 2000, 113, 5203.	1.2	72
80	Effect of basis set superposition error on the electron density of molecular complexes. Journal of Chemical Physics, 2000, 112, 10106-10115.	1.2	24
81	Theoretical study of the second-order vibrational Stark effect. Molecular Physics, 2000, 98, 513-520.	0.8	4
82	Anharmonicity contributions to the vibrational second hyperpolarizability of conjugated oligomers. Journal of Chemical Physics, 2000, 112, 1011-1019.	1.2	54
83	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.	1.1	11
84	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.	1.2	25
85	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.	1.2	82
86	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.	1.1	128
87	Theoretical Evaluation of Solvent Effects on the Conformational and Tautomeric Equilibria of 2-(2â€²-Hydroxyphenyl)benzimidazole and on Its Absorption and Fluorescence Spectra. Journal of Physical Chemistry A, 1999, 103, 4525-4532.	1.1	79
88	Weighing Different Mechanistic Proposals for the DÃ¶tz Reaction:Â A Density Functional Study. Journal of the American Chemical Society, 1999, 121, 1309-1316.	6.6	37
89	Optimizing hybrid density functionals by means of quantum molecular similarity techniques. Advances in Molecular Similarity, 1999, , 187-203.	0.5	2
90	Comparison of quantum similarity measures derived from one-electron, intracule, and extracule densities. Advances in Molecular Similarity, 1999, , 215-243.	0.5	1

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91	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.	1.0	31
92	Second-order quantum similarity measures from intracule and extracule densities. Theoretical Chemistry Accounts, 1998, 99, 44-52.	0.5	11
93	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.	0.9	24
94	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.	1.1	34
95	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.	1.2	63
96	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.	1.2	3
97	A systematic and feasible method for computing nuclear contributions to electrical properties of polyatomic molecules. Journal of Chemical Physics, 1997, 107, 1501-1512.	1.2	67
98	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.	1.2	28
99	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.	6.6	37
100	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.	1.2	54
101	How does basis set superposition error change the potential surfaces for hydrogenâ€bonded dimers?. Journal of Chemical Physics, 1996, 105, 11024-11031.	1.2	1,882
102	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
103	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
104	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.	1.0	25
105	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.	1.2	24
106	Molecular Size and Pyramidalization: Two Keys for Understanding the Reactivity of Fullerenes. The Journal of Physical Chemistry, 1995, 99, 10752-10758.	2.9	50
107	Ab initio study of the HCO 3 ? /H2O exchange in the (NH3)3 ZnII(HCO 3 ?) complex. Theoretica Chimica Acta, 1995, 91, 333-351.	0.9	1
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	Ab initio. Theoretica Chimica Acta, 1995, 91, 333.	0.9	2
110	Vibrational Stark effect and vibrational static electric properties of N2O. International Journal of Quantum Chemistry, 1994, 52, 9-15.	1.0	17
111	An AM1 study of the reactivity of buckminsterfullerene (C60) in a Diels-Alder model reaction. Chemical Physics Letters, 1994, 231, 325-330.	1.2	49
112	On the calculation ofab initioquantum molecular similarities for large systems: Fitting the electron density. Journal of Computational Chemistry, 1994, 15, 1113-1120.	1.5	46
113	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.	6.6	54
114	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
115	Intrinsic reaction coordinate of perturbed potential energy surfaces: Construction of perturbed energy profiles. International Journal of Quantum Chemistry, 1993, 47, 307-317.	1.0	1
116	Molecular electric properties and nuclear and vibrational relaxation. Molecular Physics, 1993, 80, 625-633.	0.8	67
117	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
118	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.	6.6	70
119	Valence-bond calculations on ZNO and HGO using integrals computed through the semiempiricalAM1 method. International Journal of Quantum Chemistry, 1992, 44, 887-895.	1.0	2
120	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.	0.9	16
121	Theoretical Study of the Catalyzed Hydration of CO2 by Carbonic Anhydrase: A Brief Overview.. , 1992, , 263-298.		2
122	Anion binding and pentacoordination in zinc(II) complexes. Inorganic Chemistry, 1991, 30, 2523-2527.	1.9	31
123	Analysis of solvent effects on the Menshutkin reaction. Journal of the American Chemical Society, 1991, 113, 2873-2879.	6.6	123
124	Analytic energy third derivatives for pairedâ€excited multiconfiguration selfâ€consistentâ€field wave functions. Journal of Chemical Physics, 1989, 90, 334-345.	1.2	6
125	Molecular hydrogen complex vs dihydride in ML4 + H2 systems. Influence of the ML4 fragment geometry. Inorganic Chemistry, 1989, 28, 2984-2988.	1.9	8