Eduard Matito

List of Publications by Year
in descending order

115 papers	5,299 citations	94433 37 h-index	91884 69 g-index
127 all docs	127 docs citations	127 times ranked	3149 citing authors

#	Article	IF	Citations
1	The aromatic fluctuation index (FLU): A new aromaticity index based on electron delocalization. Journal of Chemical Physics, 2005, 122, 014109.	3.0	396
2	Quantifying aromaticity with electron delocalisation measures. Chemical Society Reviews, 2015, 44, 6434-6451.	38.1	335
3	On the performance of some aromaticity indices: A critical assessment using a test set. Journal of Computational Chemistry, 2008, 29, 1543-1554.	3.3	261
4	Electron sharing indexes at the correlated level. Application to aromaticity calculations. Faraday Discussions, 2007, 135, 325-345.	3.2	203
5	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
6	Nucleus-independent chemical shift (NICS) profiles in a series of monocyclic planar inorganic compounds. Journal of Organometallic Chemistry, 2006, 691, 4359-4366.	1.8	155
7	The role of electronic delocalization in transition metal complexes from the electron localization function and the quantum theory of atoms in molecules viewpoints. Coordination Chemistry Reviews, 2009, 253, 647-665.	18.8	141
8	Electron localization function at the correlated level. Journal of Chemical Physics, 2006, 125, 024301.	3.0	135
9	Properties of Aromaticity Indices Based on the One-Electron Density Matrix. Journal of Physical Chemistry A, 2007, 111, 6521-6525.	2.5	118
10	Electron delocalization and aromaticity in low-lying excited states of archetypal organic compounds. Physical Chemistry Chemical Physics, 2011, 13, 20690.	2.8	116
11	A Critical Assessment of the Performance of Magnetic and Electronic Indices of Aromaticity. Symmetry, 2010, 2, 1156-1179.	2.2	115
12	Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. Journal of Chemical Theory and Computation, 2010, 6, 2736-2742.	5.3	115
13	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	3.3	113
14	An electronic aromaticity index for large rings. Physical Chemistry Chemical Physics, 2016, 18, 11839-11846.	2.8	110
15	Metalloaromaticity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 105-122.	14.6	105
16	Aromaticity of Distorted Benzene Rings:â€‰ Exploring the Validity of Different Indicators of Aromaticity. Journal of Physical Chemistry A, 2007, 111, 4513-4521.	2.5	102
17	New electron delocalization tools to describe the aromaticity in porphyrinoids. Physical Chemistry Chemical Physics, 2018, 20, 2787-2796.	2.8	86
18	Separation of dynamic and nondynamic correlation. Physical Chemistry Chemical Physics, 2016, 18, 24015-24023.	2.8	85

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19	A Test to Evaluate the Performance of Aromaticity Descriptors in All-Metal and Semimetal Clusters. An Appraisal of Electronic and Magnetic Indicators of Aromaticity. Journal of Chemical Theory and Computation, 2010, 6, 1118-1130.	5.3	84
20	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
21	New Solids Based on B₁₂N₁₂ Fullerenes. Journal of Physical Chemistry C, 2007, 111, 13354-13360.	3.1	72
22	On the existence and characterization of molecular electrides. Chemical Communications, 2015, 51, 4865-4868.	4.1	68
23	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
24	Allâ€Metal Antiaromaticity in Sb₄â€Type Lanthanocene Anions. Angewandte Chemie - International Edition, 2016, 55, 5531-5535.	13.8	59
25	Performance of DFT functionals for calculating the second-order nonlinear optical properties of dipolar merocyanines. Physical Chemistry Chemical Physics, 2020, 22, 16579-16594.	2.8	58
26	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
27	Peculiar Allâ€Metal Ïƒâ€Aromaticity of the [Au₂Sb₁₆]^{4â¯} Anion in the Solid State. Angewandte Chemie - International Edition, 2016, 55, 15344-15346.	13.8	52
28	Toward a Unique Definition of the Local Spin. Journal of Chemical Theory and Computation, 2012, 8, 1270-1279.	5.3	51
29	Local Descriptors of Dynamic and Nondynamic Correlation. Journal of Chemical Theory and Computation, 2017, 13, 2705-2711.	5.3	51
30	Electron delocalization and aromaticity measures within the HÃ¼ckel molecular orbital method. Computational and Theoretical Chemistry, 2007, 811, 3-11.	1.5	46
31	Electron Fluctuation in Pericyclic and Pseudopericyclic Reactions. ChemPhysChem, 2006, 7, 111-113.	2.1	45
32	Scalar and Spinâ¯Orbit Relativistic Corrections to the NICS and the Induced Magnetic Field: The case of the E₁₂^{2â¯} Spherenes (E = Ge, Sn, Pb). Journal of Chemical Theory and Computation, 2010, 6, 2701-2705.	5.3	44
33	Oï¿O Bond Formation Mediated by a Hexanuclear Iron Complex Supported on a Stannoxane Core. Chemistry - A European Journal, 2012, 18, 2787-2791.	3.3	44
34	Tuning aromaticity in trigonal alkaline earth metal clusters and their alkali metal salts. Journal of Computational Chemistry, 2009, 30, 2764-2776.	3.3	43
35	How do the HÃ¼ckel and Baird Rules Fade away in Annulenes?. Molecules, 2020, 25, 711.	3.8	43
36	Bonding in Methylalkalimetals (CH3M)n(M = Li, Na, K;n= 1, 4). Agreement and Divergences between AIM and ELF Analysesâ€. Journal of Physical Chemistry B, 2006, 110, 7189-7198.	2.6	39

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37	Using Electronic Energy Derivative Information in Automated Potential Energy Surface Construction for Vibrational Calculations. Journal of Chemical Theory and Computation, 2010, 6, 3162-3175.	5.3	39
38	Analysis of HÃ¼ckelâ€™s [4n+ 2] Rule through Electronic Delocalization Measures. Journal of Physical Chemistry A, 2008, 112, 13231-13238.	2.5	38
39	Patterns of Ï€-electron delocalization in aromatic and antiaromatic organic compounds in the light of HÃ¼ckel's 4n + 2 rule. Physical Chemistry Chemical Physics, 2010, 12, 7126.	2.8	38
40	How Aromatic Are Molecular Nanorings? The Case of a Sixâ€Porphyrin Nanoring**. Angewandte Chemie - International Edition, 2021, 60, 24080-24088.	13.8	38
41	A theoretical study of the aromaticity in neutral and anionic borole compounds. Dalton Transactions, 2015, 44, 6740-6747.	3.3	37
42	Comprehensive benchmarking of density matrix functional approximations. Physical Chemistry Chemical Physics, 2017, 19, 24029-24041.	2.8	37
43	Performance of 3Dâ€spaceâ€based atomsâ€inâ€molecules methods for electronic delocalization aromaticity indices. Journal of Computational Chemistry, 2011, 32, 386-395.	3.3	36
44	The aromaticity of dicupra[10]annulenes. Physical Chemistry Chemical Physics, 2017, 19, 9669-9675.	2.8	33
45	Overcoming the Failure of Correlation for Out-of-Plane Motions in a Simple Aromatic: Rovibrational Quantum Chemical Analysis ofc-C₃H₂. Journal of Chemical Theory and Computation, 2018, 14, 2155-2164.	5.3	33
46	Properties of harmonium atoms from FCI calculations: Calibration and benchmarks for the ground state of the two-electron species. Physical Chemistry Chemical Physics, 2010, 12, 6712.	2.8	31
47	New Approximation to the Third-Order Density. Application to the Calculation of Correlated Multicenter Indices. Journal of Chemical Theory and Computation, 2014, 10, 3055-3065.	5.3	31
48	A hierarchy of potential energy surfaces constructed from energies and energy derivatives calculated on grids. Journal of Chemical Physics, 2009, 130, 134104.	3.0	30
49	Understanding Conjugation and Hyperconjugation from Electronic Delocalization Measures. Journal of Physical Chemistry A, 2011, 115, 13104-13113.	2.5	30
50	New Link between Conceptual Density Functional Theory and Electron Delocalization. Journal of Physical Chemistry A, 2011, 115, 12459-12462.	2.5	30
51	Local spins: improved Hilbert-space analysis. Physical Chemistry Chemical Physics, 2012, 14, 15291.	2.8	30
52	Vibrational coupled cluster theory with full two-mode and approximate three-mode couplings: The VCC[2pt3] model. Journal of Chemical Physics, 2009, 131, 034115.	3.0	29
53	Exploring the Relation Between Intramolecular Conjugation and Band Dispersion in One-Dimensional Polymers. Journal of Physical Chemistry C, 2017, 121, 27118-27125.	3.1	29
54	Analysis of Electron Delocalization in Aromatic Systems:â€‰ Individual Molecular Orbital Contributions to Para-Delocalization Indexes (PDI). Journal of Physical Chemistry A, 2006, 110, 11569-11574.	2.5	28

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55	Robust validation of approximate 1-matrix functionals with few-electron harmonium atoms. Journal of Chemical Physics, 2015, 143, 214101.	3.0	28
56	Metal Cluster Electrides: A New Type of Molecular Electride with Delocalised Polyattractor Character. Chemistry - A European Journal, 2018, 24, 9853-9859.	3.3	28
57	Singling Out Dynamic and Nondynamic Correlation. Journal of Physical Chemistry Letters, 2019, 10, 4032-4037.	4.6	28
58	A new tuned range-separated density functional for the accurate calculation of second hyperpolarizabilities. Physical Chemistry Chemical Physics, 2020, 22, 11871-11880.	2.8	28
59	The three-electron harmonium atom: The lowest-energy doublet and quadruplet states. Journal of Chemical Physics, 2012, 136, 194112.	3.0	27
60	Benchmark calculations on the lowest-energy singlet, triplet, and quintet states of the four-electron harmonium atom. Journal of Chemical Physics, 2014, 141, 044128.	3.0	26
61	Choosing Bad versus Worse: Predictions of Two-Photon-Absorption Strengths Based on Popular Density Functional Approximations. Journal of Chemical Theory and Computation, 2022, 18, 1046-1060.	5.3	26
62	Performance of PNOF5 Natural Orbital Functional for Radical Formation Reactions: Hydrogen Atom Abstraction and Câ€“C and Oâ€“O Homolytic Bond Cleavage in Selected Molecules. Journal of Chemical Theory and Computation, 2012, 8, 2646-2652.	5.3	24
63	The Electronic Structure of the Al₃^{â^’} Anion: Is it Aromatic?. Chemistry - A European Journal, 2015, 21, 9610-9614.	3.3	23
64	Calculation of local spins for correlated wave functions. Physical Chemistry Chemical Physics, 2010, 12, 11308.	2.8	22
65	All-metal Ï*f*-antiaromaticity in dimeric cluster anion {[CuGe₉Mes]₂}^{4â^’}. Chemical Communications, 2020, 56, 6583-6586.	4.1	22
66	Approximate Inclusion of Triple Excitations in Combined Coupled Cluster/Molecular Mechanics: Calculations of Electronic Excitation Energies in Solution for Acrolein, Water, Formamide, and N-Methylacetamide. Journal of Chemical Theory and Computation, 2010, 6, 839-850.	5.3	21
67	H4: A challenging system for natural orbital functional approximations. Journal of Chemical Physics, 2015, 143, 164112.	3.0	21
68	Can Density Functional Theory Be Trusted for High-Order Electric Properties? The Case of Hydrogen-Bonded Complexes. Journal of Chemical Theory and Computation, 2019, 15, 3570-3579.	5.3	21
69	Ab Initio Design of Chelating Ligands Relevant to Alzheimerâ€™s Disease: Influence of Metalloaromaticity. Journal of Physical Chemistry A, 2011, 115, 12659-12666.	2.5	20
70	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
71	Exploring the Potential Energy Surface of E₂P₄ Clusters (E=Groupâ€…13 Element): The Quest for Inverse Carbonâ€Free Sandwiches. Chemistry - A European Journal, 2014, 20, 4583-4590.	3.3	19
72	Peculiar Allâ€Metal Ïâ€Aromaticity of the [Au₂Sb₁₆]^{4â^’} Anion in the Solid State. Angewandte Chemie, 2016, 128, 15570-15572.	2.0	19

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73	Molecular structures of M2N22â^' (M and N = B, Al, and Ga) clusters using the gradient embedded genetic algorithm. Physical Chemistry Chemical Physics, 2012, 14, 14850.	2.8	18
74	Transitionâ€Metal Ï€â€Ligation of a Tetrahalodiborane. Angewandte Chemie - International Edition, 2018, 57, 412-416.	13.8	18
75	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
76	Benchmark Full Configuration Interaction Calculations on the Lowest-Energy ²P and ⁴P States of the Three-Electron Harmonium Atom. Journal of Chemical Theory and Computation, 2011, 7, 915-920.	5.3	17
77	Two new constraints for the cumulant matrix. Journal of Chemical Physics, 2014, 141, 234101.	3.0	17
78	Fermi and Coulomb correlation effects upon the interacting quantum atoms energy partition. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	17
79	Guidelines for Tuning the Excited State HÃ¼ckelâ€“Baird Hybrid Aromatic Character of Proâ€Aromatic Quinoidal Compounds**. Angewandte Chemie - International Edition, 2021, 60, 10255-10265.	13.8	17
80	Tuning the affinity of catechols and salicylic acids towards Al(<scp>iii</scp>): characterization of Alâ€“chelator interactions. Dalton Transactions, 2018, 47, 9592-9607.	3.3	14
81	Impact of van der Waals interactions on the structural and nonlinear optical properties of azobenzene switches. Physical Chemistry Chemical Physics, 2021, 23, 21227-21239.	2.8	14
82	Bonding description of the Harpoon mechanism. Molecular Physics, 2016, 114, 1345-1355.	1.7	13
83	Electron correlation effects in third-order densities. Physical Chemistry Chemical Physics, 2017, 19, 4522-4529.	2.8	13
84	Aromaticity descriptors based on electron delocalization. , 2021, , 235-259.		13
85	Note: The weak-correlation limit of the three-electron harmonium atom. Journal of Chemical Physics, 2011, 134, 116101.	3.0	12
86	How Reliable Are Modern Density Functional Approximations to Simulate Vibrational Spectroscopies?. Journal of Physical Chemistry Letters, 2022, 13, 5963-5968.	4.6	12
87	Allâ€Metal Antiaromaticity in Sb₄â€Type Lanthanocene Anions. Angewandte Chemie, 2016, 128, 5621-5625.	2.0	11
88	Salient signature of van der Waals interactions. Physical Review A, 2017, 96, .	2.5	10
89	Benchmark calculations of metal carbonyl cations: relativistic vs. electron correlation effects. Physical Chemistry Chemical Physics, 2013, 15, 20080.	2.8	9
90	Cycloreversion of the CO₂trimer: a paradigmatic pseudopericyclic [2 + 2 + 2] cycloaddition reaction. Organic and Biomolecular Chemistry, 2017, 15, 435-441.	2.8	9

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91	The vibrational auto-adjusting perturbation theory. Theoretical Chemistry Accounts, 2009, 123, 41-49.	1.4	8
92	Three-center bonding analyzed from correlated and uncorrelated third-order reduced density matrices. Computational and Theoretical Chemistry, 2015, 1053, 173-179.	2.5	8
93	Reply to the Correspondence on â€œHow Aromatic Are Molecular Nanorings? The Case of a Sixâ€Porphyrin Nanoringâ€**. Angewandte Chemie - International Edition, 2022, 61, .	13.8	8
94	Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. Journal of Chemical Theory and Computation, 2011, 7, 1231-1231.	5.3	7
95	Rules of Aromaticity. Challenges and Advances in Computational Chemistry and Physics, 2016, , 321-335.	0.6	7
96	Ãœbergangsmetallâ€Ïâ€Komplexierung eines Tetrahalogendiborans. Angewandte Chemie, 2018, 130, 419-423.	2.0	7
97	How Many Electrons Does a Molecular Electride Hold?. Journal of Physical Chemistry A, 2021, 125, 4819-4835.	2.5	7
98	How Aromatic Are Molecular Nanorings? The Case of a Sixâ€Porphyrin Nanoring**. Angewandte Chemie, 2021, 133, 24282.	2.0	7
99	Bond centred functions in relativistic and non-relativistic calculations for diatomics. Chemical Physics, 2006, 321, 277-284.	1.9	6
100	Aromaticity Analysis by Means of the Quantum Theory of Atoms in Molecules. , 0, , 399-423.		6
101	Electron-Pair Distribution in Chemical Bond Formation. Journal of Physical Chemistry A, 2018, 122, 1916-1923.	2.5	6
102	The electronic structure and stability of germanium tubes Ge₃₀H₁₂ and Ge₃₃H₁₂. Physical Chemistry Chemical Physics, 2018, 20, 23467-23479.	2.8	6
103	The Coulomb Hole of the Ne Atom. ChemistryOpen, 2019, 8, 411-417.	1.9	6
104	The electron-pair density distribution of the^{1,3}Î_uexcited states of H₂. Canadian Journal of Chemistry, 2016, 94, 998-1001.	1.1	5
105	Partition of optical properties into orbital contributions. Physical Chemistry Chemical Physics, 2019, 21, 15380-15391.	2.8	5
106	Aromaticity and Chemical Reactivity. , 2009, , .		5
107	Guidelines for Tuning the Excited State HÃ¼ckelâ€“Baird Hybrid Aromatic Character of Proâ€Aromatic Quinoidal Compounds**. Angewandte Chemie, 2021, 133, 10343-10353.	2.0	3
108	Natural range separation of the Coulomb hole. Journal of Chemical Physics, 2022, 156, 184106.	3.0	3

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109	Comment to â€˜A new population analysis: Dipole-moment-conserving charge-setâ€™ by H. Sato, S. Skaki [Chem. Phys. Lett. 434 (2007) 165]. Chemical Physics Letters, 2008, 451, 169-170.	2.6	0
110	Editorial [Hot Topic: Electron Delocalization in Organic Chemistry (Guest Editors: Dr. Eduard Matito) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	1.6	0
111	Exploring the Potential Energy Surface of E2P4Clusters (E=Groupâ€…13 Element): The Quest for Inverse Carbon-Free Sandwiches. Chemistry - A European Journal, 2014, 20, 4497-4497.	3.3	0
112	Frontispiece: The Electronic Structure of the Al3â¯Anion: Is it Aromatic?. Chemistry - A European Journal, 2015, 21, n/a-n/a.	3.3	0
113	Frontispiece: How Aromatic Are Molecular Nanorings? The Case of a Sixâ€Porphyrin Nanoring. Angewandte Chemie - International Edition, 2021, 60, .	13.8	0
114	Frontispiz: How Aromatic Are Molecular Nanorings? The Case of a Sixâ€Porphyrin Nanoring. Angewandte Chemie, 2021, 133, .	2.0	0
115	Reply to the Correspondence on â€œHow Aromatic Are Molecular Nanorings? The Case of a Sixâ€Porphyrin Nanoringâ€**. Angewandte Chemie, 0, , .	2.0	0