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	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
2	Natural range separation of the Coulomb hole. Journal of Chemical Physics, 2022, 156, 184106.	3.0	3
3	How Reliable Are Modern Density Functional Approximations to Simulate Vibrational Spectroscopies?. Journal of Physical Chemistry Letters, 2022, 13, 5963-5968.	4.6	12
4	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
5	Aromaticity descriptors based on electron delocalization. , 2021, , 235-259.		13
6	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
7	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
8	How Many Electrons Does a Molecular Electride Hold?. Journal of Physical Chemistry A, 2021, 125, 4819-4835.	2.5	7
9	How Aromatic Are Molecular Nanorings? The Case of a Sixâ€Porphyrin Nanoring**. Angewandte Chemie - International Edition, 2021, 60, 24080-24088.	13.8	38
10	How Aromatic Are Molecular Nanorings? The Case of a Sixâ€Porphyrin Nanoring**. Angewandte Chemie, 2021, 133, 24282.	2.0	7
11	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
12	Frontispiece: How Aromatic Are Molecular Nanorings? The Case of a Sixâ€Porphyrin Nanoring. Angewandte Chemie - International Edition, 2021, 60, .	13.8	0
13	Frontispiz: How Aromatic Are Molecular Nanorings? The Case of a Sixâ€Porphyrin Nanoring. Angewandte Chemie, 2021, 133, .	2.0	0
14	All-metal Ï*f*-antiaromaticity in dimeric cluster anion {[CuGe₉Mes]₂}^{4â^'}. Chemical Communications, 2020, 56, 6583-6586.	4.1	22
15	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
16	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
17	How do the HÃ¼ckel and Baird Rules Fade away in Annulenes?. Molecules, 2020, 25, 711.	3.8	43
18	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	3.3	113

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19	Partition of optical properties into orbital contributions. Physical Chemistry Chemical Physics, 2019, 21, 15380-15391.	2.8	5
20	Singling Out Dynamic and Nondynamic Correlation. Journal of Physical Chemistry Letters, 2019, 10, 4032-4037.	4.6	28
21	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
22	The Coulomb Hole of the Ne Atom. ChemistryOpen, 2019, 8, 411-417.	1.9	6
23	Metal Cluster Electrides: A New Type of Molecular Electride with Delocalised Polyattractor Character. Chemistry - A European Journal, 2018, 24, 9853-9859.	3.3	28
24	Electron-Pair Distribution in Chemical Bond Formation. Journal of Physical Chemistry A, 2018, 122, 1916-1923.	2.5	6
25	New electron delocalization tools to describe the aromaticity in porphyrinoids. Physical Chemistry Chemical Physics, 2018, 20, 2787-2796.	2.8	86
26	Ãœbergangsmetallâ€Ïâ€Komplexierung eines Tetrahalogendiborans. Angewandte Chemie, 2018, 130, 419-423.	2.0	7
27	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
28	Transitionâ€Metal Ïâ€Ligation of a Tetrahalodiborane. Angewandte Chemie - International Edition, 2018, 57, 412-416.	13.8	18
29	The electronic structure and stability of germanium tubes Ge₃₀H₁₂ and Ge₃₃H₁₂. Physical Chemistry Chemical Physics, 2018, 20, 23467-23479.	2.8	6
30	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
31	Electron correlation effects in third-order densities. Physical Chemistry Chemical Physics, 2017, 19, 4522-4529.	2.8	13
32	Local Descriptors of Dynamic and Nondynamic Correlation. Journal of Chemical Theory and Computation, 2017, 13, 2705-2711.	5.3	51
33	The aromaticity of dicupra[10]annulenes. Physical Chemistry Chemical Physics, 2017, 19, 9669-9675.	2.8	33
34	Cycloreversion of the CO₂trimer: a paradigmatic pseudopericyclic [2 + 2 + 2] cycloaddition reaction. Organic and Biomolecular Chemistry, 2017, 15, 435-441.	2.8	9
35	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
36	Comprehensive benchmarking of density matrix functional approximations. Physical Chemistry Chemical Physics, 2017, 19, 24029-24041.	2.8	37

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37	Salient signature of van der Waals interactions. Physical Review A, 2017, 96, .	2.5	10
38	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
39	Allâ€Metal Antiaromaticity in Sb₄â€Type Lanthanocene Anions. Angewandte Chemie, 2016, 128, 5621-5625.	2.0	11
40	Rules of Aromaticity. Challenges and Advances in Computational Chemistry and Physics, 2016, , 321-335.	0.6	7
41	Fermi and Coulomb correlation effects upon the interacting quantum atoms energy partition. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	17
42	Separation of dynamic and nondynamic correlation. Physical Chemistry Chemical Physics, 2016, 18, 24015-24023.	2.8	85
43	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
44	Peculiar Allâ€Metal Ïƒâ€Aromaticity of the [Au₂Sb₁₆]^{4â^'} Anion in the Solid State. Angewandte Chemie, 2016, 128, 15570-15572.	2.0	19
45	Allâ€Metal Antiaromaticity in Sb₄â€Type Lanthanocene Anions. Angewandte Chemie - International Edition, 2016, 55, 5531-5535.	13.8	59
46	Bonding description of the Harpoon mechanism. Molecular Physics, 2016, 114, 1345-1355.	1.7	13
47	An electronic aromaticity index for large rings. Physical Chemistry Chemical Physics, 2016, 18, 11839-11846.	2.8	110
48	Robust validation of approximate 1-matrix functionals with few-electron harmonium atoms. Journal of Chemical Physics, 2015, 143, 214101.	3.0	28
49	H4: A challenging system for natural orbital functional approximations. Journal of Chemical Physics, 2015, 143, 164112.	3.0	21
50	Frontispiece: The Electronic Structure of the Al3â^'Anion: Is it Aromatic?. Chemistry - A European Journal, 2015, 21, n/a-n/a.	3.3	0
51	The Electronic Structure of the Al₃^{â^'} Anion: Is it Aromatic?. Chemistry - A European Journal, 2015, 21, 9610-9614.	3.3	23
52	Three-center bonding analyzed from correlated and uncorrelated third-order reduced density matrices. Computational and Theoretical Chemistry, 2015, 1053, 173-179.	2.5	8
53	On the existence and characterization of molecular electrides. Chemical Communications, 2015, 51, 4865-4868.	4.1	68
54	Quantifying aromaticity with electron delocalisation measures. Chemical Society Reviews, 2015, 44, 6434-6451.	38.1	335

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55	A theoretical study of the aromaticity in neutral and anionic borole compounds. Dalton Transactions, 2015, 44, 6740-6747.	3.3	37
56	Two new constraints for the cumulant matrix. Journal of Chemical Physics, 2014, 141, 234101.	3.0	17
57	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
58	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
59	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
60	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
61	Benchmark calculations of metal carbonyl cations: relativistic vs. electron correlation effects. Physical Chemistry Chemical Physics, 2013, 15, 20080.	2.8	9
62	Metalloaromaticity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 105-122.	14.6	105
63	The three-electron harmonium atom: The lowest-energy doublet and quadruplet states. Journal of Chemical Physics, 2012, 136, 194112.	3.0	27
64	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
65	Local spins: improved Hilbert-space analysis. Physical Chemistry Chemical Physics, 2012, 14, 15291.	2.8	30
66	Toward a Unique Definition of the Local Spin. Journal of Chemical Theory and Computation, 2012, 8, 1270-1279.	5.3	51
67	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
68	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
69	Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. Journal of Chemical Theory and Computation, 2011, 7, 1231-1231.	5.3	7
70	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
71	Understanding Conjugation and Hyperconjugation from Electronic Delocalization Measures. Journal of Physical Chemistry A, 2011, 115, 13104-13113.	2.5	30
72	New Link between Conceptual Density Functional Theory and Electron Delocalization. Journal of Physical Chemistry A, 2011, 115, 12459-12462.	2.5	30

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73	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
74	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
75	Electron delocalization and aromaticity in low-lying excited states of archetypal organic compounds. Physical Chemistry Chemical Physics, 2011, 13, 20690.	2.8	116
76	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
77	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
78	Note: The weak-correlation limit of the three-electron harmonium atom. Journal of Chemical Physics, 2011, 134, 116101.	3.0	12
79	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
80	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
81	A Critical Assessment of the Performance of Magnetic and Electronic Indices of Aromaticity. Symmetry, 2010, 2, 1156-1179.	2.2	115
82	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
83	Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. Journal of Chemical Theory and Computation, 2010, 6, 2736-2742.	5.3	115
84	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
85	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
86	Calculation of local spins for correlated wave functions. Physical Chemistry Chemical Physics, 2010, 12, 11308.	2.8	22
87	Scalar and Spinâ^'Orbit Relativistic Corrections to the NICS and the Induced Magnetic Field: The case of the E‹sub›12‹/sub›‹sup›2â^'‹/sup› Spherenes (E = Ge, Sn, Pb). Journal of Chemical Theory and Computation, 2010, 6, 2701-2705.	5.3	44
88	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
89	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
90	Tuning aromaticity in trigonal alkaline earth metal clusters and their alkali metal salts. Journal of Computational Chemistry, 2009, 30, 2764-2776.	3.3	43

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91	The vibrational auto-adjusting perturbation theory. Theoretical Chemistry Accounts, 2009, 123, 41-49.	1.4	8
92	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
93	Aromaticity and Chemical Reactivity. , 2009, , .		5
94	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
95	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
96	Analysis of HÃ¼ckelâ€™s [4n+ 2] Rule through Electronic Delocalization Measures. Journal of Physical Chemistry A, 2008, 112, 13231-13238.	2.5	38
97	New Solids Based on B₁₂N₁₂ Fullerenes. Journal of Physical Chemistry C, 2007, 111, 13354-13360.	3.1	72
98	Electron sharing indexes at the correlated level. Application to aromaticity calculations. Faraday Discussions, 2007, 135, 325-345.	3.2	203
99	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
100	Properties of Aromaticity Indices Based on the One-Electron Density Matrix. Journal of Physical Chemistry A, 2007, 111, 6521-6525.	2.5	118
101	Electron delocalization and aromaticity measures within the HÃ¼ckel molecular orbital method. Computational and Theoretical Chemistry, 2007, 811, 3-11.	1.5	46
102	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
103	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
104	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
105	Electron localization function at the correlated level. Journal of Chemical Physics, 2006, 125, 024301.	3.0	135
106	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
107	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
108	Bond centred functions in relativistic and non-relativistic calculations for diatomics. Chemical Physics, 2006, 321, 277-284.	1.9	6

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109	Electron Fluctuation in Pericyclic and Pseudopericyclic Reactions. ChemPhysChem, 2006, 7, 111-113.	2.1	45
110	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
111	The aromatic fluctuation index (FLU): A new aromaticity index based on electron delocalization. Journal of Chemical Physics, 2005, 122, 014109.	3.0	396
112	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
113	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
114	Aromaticity Analysis by Means of the Quantum Theory of Atoms in Molecules. , 0, , 399-423.		6
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