Ferran Feixas

List of Publications by Year
in descending order

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53 papers	2,641 citations	201674 27 h-index	182427 51 g-index
59 all docs	59 docs citations	59 times ranked	2980 citing authors

#	Article	IF	Citations
1	Quantifying aromaticity with electron delocalisation measures. Chemical Society Reviews, 2015, 44, 6434-6451.	38.1	335
2	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
3	Accelerated molecular dynamics simulations of protein folding. Journal of Computational Chemistry, 2015, 36, 1536-1549.	3.3	134
4	Exploring the role of receptor flexibility in structure-based drug discovery. Biophysical Chemistry, 2014, 186, 31-45.	2.8	129
5	Intrinsic enzymatic properties modulate the self-propulsion of micromotors. Nature Communications, 2019, 10, 2826.	12.8	126
6	Electron delocalization and aromaticity in low-lying excited states of archetypal organic compounds. Physical Chemistry Chemical Physics, 2011, 13, 20690.	2.8	116
7	A Critical Assessment of the Performance of Magnetic and Electronic Indices of Aromaticity. Symmetry, 2010, 2, 1156-1179.	2.2	115
8	Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. Journal of Chemical Theory and Computation, 2010, 6, 2736-2742.	5.3	115
9	Metalloaromaticity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 105-122.	14.6	105
10	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
11	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
12	p38Î³ is essential for cell cycle progression and liver tumorigenesis. Nature, 2019, 568, 557-560.	27.8	72
13	Unraveling factors leading to efficient norbornadieneâ€“quadricyclane molecular solar-thermal energy storage systems. Journal of Materials Chemistry A, 2017, 5, 12369-12378.	10.3	65
14	A dissected ring current model for assessing magnetic aromaticity: A general approach for both organic and inorganic rings. Journal of Computational Chemistry, 2011, 32, 2422-2431.	3.3	61
15	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
16	Electron delocalization and aromaticity measures within the HÃ¼ckel molecular orbital method. Computational and Theoretical Chemistry, 2007, 811, 3-11.	1.5	46
17	Undecaprenyl Diphosphate Synthase Inhibitors: Antibacterial Drug Leads. Journal of Medicinal Chemistry, 2014, 57, 5693-5701.	6.4	43
18	Analysis of HÃ¼ckelâ€™s [4n+ 2] Rule through Electronic Delocalization Measures. Journal of Physical Chemistry A, 2008, 112, 13231-13238.	2.5	38

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19	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
20	Complete Dynamic Reconstruction of C₆₀, C₇₀, and (C₅₉N)₂ Encapsulation into an Adaptable Supramolecular Nanocapsule. Journal of the American Chemical Society, 2020, 142, 16051-16063.	13.7	36
21	Ultrafast irreversible phototautomerization of o-nitrobenzaldehyde. Chemical Communications, 2011, 47, 6383.	4.1	33
22	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
23	Electronic States of o-Nitrobenzaldehyde: A Combined Experimental and Theoretical Study. Journal of Physical Chemistry A, 2008, 112, 5046-5053.	2.5	30
24	Understanding Conjugation and Hyperconjugation from Electronic Delocalization Measures. Journal of Physical Chemistry A, 2011, 115, 13104-13113.	2.5	30
25	Analysis of a Compound Class with Triplet States Stabilized by Potentially Baird Aromatic [10]Annulenyl Dicationic Rings. Chemistry - A European Journal, 2016, 22, 2793-2800.	3.3	30
26	Peculiarities of Multiple Crâ‹¯Cr Bonding. Insights from the Analysis of Domain-Averaged Fermi Holes. Journal of Physical Chemistry A, 2009, 113, 8394-8400.	2.5	28
27	Metal Cluster Electrides: A New Type of Molecular Electride with Delocalised Polyattractor Character. Chemistry - A European Journal, 2018, 24, 9853-9859.	3.3	28
28	Toward Bioelectronic Nanomaterials: Photoconductivity in Proteinâ€“Porphyrin Hybrids Wrapped around SWCNT. Advanced Functional Materials, 2018, 28, 1704031.	14.9	25
29	Exploring the validity of the Glidewellâ€“Lloyd extension of Clarâ€™s Ï€-sextet rule: assessment from polycyclic conjugated hydrocarbons. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	24
30	Time Evolution of the Millisecond Allosteric Activation of Imidazole Glycerol Phosphate Synthase. Journal of the American Chemical Society, 2022, 144, 7146-7159.	13.7	24
31	Interplay between R513 methylation and S516 phosphorylation of the cardiac voltage-gated sodium channel. Amino Acids, 2015, 47, 429-434.	2.7	23
32	Machine Learning Enables Selection of Epistatic Enzyme Mutants for Stability Against Unfolding and Detrimental Aggregation. ChemBioChem, 2021, 22, 904-914.	2.6	22
33	Discovery and In Vivo Proof of Concept of a Highly Potent Dual Inhibitor of Soluble Epoxide Hydrolase and Acetylcholinesterase for the Treatment of Alzheimerâ€™s Disease. Journal of Medicinal Chemistry, 2022, 65, 4909-4925.	6.4	22
34	Hidden Conformations in Aspergillus niger Monoamine Oxidase are Key for Catalytic Efficiency. Angewandte Chemie - International Edition, 2019, 58, 3097-3101.	13.8	18
35	A non-adiabatic quantum-classical dynamics study of the intramolecular excited state hydrogen transfer in ortho-nitrobenzaldehyde. Physical Chemistry Chemical Physics, 2011, 13, 14685.	2.8	17
36	All-metal aromatic clusters M42â‹¯ (M = B, Al, and Ga). Are Ï€-electrons distortive or not?. Physical Chemistry Chemical Physics, 2011, 13, 20673.	2.8	14

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37	A Molecular Dynamics Investigation of Mycobacterium tuberculosis Prenyl Synthases: Conformational Flexibility and Implications for Computerâ€aided Drug Discovery. Chemical Biology and Drug Design, 2015, 85, 756-769.	3.2	14
38	2-Oxaadamant-1-yl Ureas as Soluble Epoxide Hydrolase Inhibitors: In Vivo Evaluation in a Murine Model of Acute Pancreatitis. Journal of Medicinal Chemistry, 2020, 63, 9237-9257.	6.4	14
39	Electron correlation effects in third-order densities. Physical Chemistry Chemical Physics, 2017, 19, 4522-4529.	2.8	13
40	Octahedral aromaticity in ^{2S+1}A_{1g} X₆^q clusters (X =) Tj ETQq0 0 0 rgBT /Overlock	2.8	12
41	From the Design to the In Vivo Evaluation of Benzohomoadamantane-Derived Soluble Epoxide Hydrolase Inhibitors for the Treatment of Acute Pancreatitis. Journal of Medicinal Chemistry, 2021, 64, 5429-5446.	6.4	12
42	Protein-directed crystalline 2D fullerene assemblies. Nanoscale, 2020, 12, 3614-3622.	5.6	11
43	Domain Averaged Fermi Hole Analysis for Open-Shell Systems. Journal of Physical Chemistry A, 2009, 113, 5773-5779.	2.5	9
44	Three-center bonding analyzed from correlated and uncorrelated third-order reduced density matrices. Computational and Theoretical Chemistry, 2015, 1053, 173-179.	2.5	8
45	Epoxide Hydrolase Conformational Heterogeneity for the Resolution of Bulky Pharmacologically Relevant Epoxide Substrates. Chemistry - A European Journal, 2018, 24, 12254-12258.	3.3	8
46	Bonding Analysis of the [C₂O₄]²⁺ Intermediate Formed in the Reaction of CO₂²⁺ with Neutral CO₂. Journal of Physical Chemistry A, 2010, 114, 6681-6688.	2.5	7
47	Electron Localization Function at the Correlated Level: A Natural Orbital Formulation. Journal of Chemical Theory and Computation, 2011, 7, 1231-1231.	5.3	7
48	Rules of Aromaticity. Challenges and Advances in Computational Chemistry and Physics, 2016, , 321-335.	0.6	7
49	Comprehensive Characterization of the Selfâ€Folding Cavitand Dynamics. Chemistry - A European Journal, 2021, 27, 10099-10106.	3.3	5
50	Molecular Dynamics Simulations on Aspergillus niger Monoamine Oxidase: Conformational Dynamics and Interâ€monomer Communication Essential for Its Efficient Catalysis. Advanced Synthesis and Catalysis, 2019, 361, 2718.	4.3	3
51	Changes in Protonation States of In-Pathway Residues can Alter Ligand Binding Pathways Obtained From Spontaneous Binding Molecular Dynamics Simulations. Frontiers in Molecular Biosciences, 0, 9, .	3.5	2
52	Accelerated Molecular Dynamics Simulations of Protein Folding. Journal of Computational Chemistry, 2016, 37, .	3.3	1
53	Hidden Conformations in Aspergillus niger Monoamine Oxidase are Key for Catalytic Efficiency. Angewandte Chemie, 2019, 131, 3129-3133.	2.0	0