Alejandro Morales-Bayuelo

List of Publications by Year
in descending order

60	710	567281 15	713466 21
papers	citations	h-index	g-index

60	60	60	311
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The response of the electronic structure to electronic excitation and double bond torsion in fulvene: a combined QTAIM, stress tensor and MO perspective. Physical Chemistry Chemical Physics, 2014, 16, 7115-7126.	2.8	58
2	Biphenyl: A stress tensor and vector-based perspective explored within the quantum theory of atoms in molecules. International Journal of Quantum Chemistry, 2015, 115, 1678-1690.	2.0	46
3	Distinguishing and quantifying the torquoselectivity in competitive ring-opening reactions using the stress tensor and QTAIM. Journal of Computational Chemistry, 2016, 37, 2722-2733.	3.3	38
4	Topological model to quantify the global reactivity indexes as local in Dielsâ€“Alder reactions, using density function theory (DFT) and local quantum similarity (LQS). Journal of Mathematical Chemistry, 2013, 51, 125-143.	1.5	24
5	Fatigue and photochromism S₁ excited state reactivity of diarylethenes from QTAIM and the stress tensor. International Journal of Quantum Chemistry, 2018, 118, e25565.	2.0	23
6	Stress tensor eigenvector following with nextâ€generation quantum theory of atoms in molecules. International Journal of Quantum Chemistry, 2019, 119, e25847.	2.0	23
7	Quinoneâ€based switches for candidate building blocks of molecular junctions with QTAIM and the stress tensor. International Journal of Quantum Chemistry, 2018, 118, e25676.	2.0	21
8	Intramolecular mode coupling of the isotopomers of water: a non-scalar charge density-derived perspective. Physical Chemistry Chemical Physics, 2020, 22, 2509-2520.	2.8	19
9	HÃœCKEL TREATMENT OF PYRROLE AND PENTALENE AS A FUNCTION OF CYCLOPENTADIENYL USING LOCAL QUANTUM SIMILARITY INDEX (LQSI) AND THE TOPO-GEOMETRICAL SUPERPOSITION APPROACH (TGSA). Journal of Theoretical and Computational Chemistry, 2012, 11, 223-239.	1.8	18
10	Nextâ€generation quantum theory of atoms in molecules for the ground and excited states of fulvene. International Journal of Quantum Chemistry, 2018, 118, e25768.	2.0	18
11	Nextâ€generation quantum theory of atoms in molecules for the ground and excited state of the ringâ€opening of cyclohexadiene. International Journal of Quantum Chemistry, 2019, 119, e25862.	2.0	18
12	Theoretical study of the chemical reactivity and molecular quantum similarity in a series of derivatives of 2â€adamantylâ€thiazolidineâ€4â€one using density functional theory and the topoâ€geometrical superposition approach. International Journal of Quantum Chemistry, 2012, 112, 2681-2687.	2.0	17
13	Understanding the electronic reorganization in the thermal isomerization reaction of transâ€3,4â€dimethylcyclobutene. Origins of outward Pseudodiradical {2n + 2Ï€} torquoselectivity. International Journal of Quantum Chemistry, 2013, 113, 1534-1543.	2.0	17
14	A bond, ring and cage resolved PoincarÃ©â€“Hopf relationship for isomerisation reaction pathways. Molecular Physics, 2013, 111, 3104-3116.	1.7	17
15	Analyzing torquoselectivity in electrocyclic ring opening reactions of trans-3,4-dimethylcyclobutene and 3-formylcyclobutene through electronic structure principles. Physical Chemistry Chemical Physics, 2015, 17, 23104-23111.	2.8	17
16	QTAIM and Stress Tensor Characterization of Intramolecular Interactions Along Dynamics Trajectories of a Light-Driven Rotary Molecular Motor. Journal of Physical Chemistry A, 2017, 121, 4778-4792.	2.5	17
17	A QTAIM and stress tensor investigation of the torsion path of a light-driven fluorene molecular rotary motor. Journal of Computational Chemistry, 2016, 37, 2588-2596.	3.3	15
18	The destabilization of hydrogen bonds in an external Eâ€field for improved switch performance. Journal of Computational Chemistry, 2019, 40, 1881-1891.	3.3	15

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19	The cis-effect using the topology of the electronic charge density. Molecular Physics, 2013, 111, 793-805.	1.7	14
20	Quantum molecular similarity analysis and quantitative definition of catecholamines with respect to biogenic monoamines associated: Scale alpha and beta of quantitative convergence. International Journal of Quantum Chemistry, 2012, 112, 2637-2642.	2.0	12
21	Nextâ€generation quantum theory of atoms in molecules for the photochemical ringâ€opening reactions of oxirane. International Journal of Quantum Chemistry, 2019, 119, e25957.	2.0	12
22	Nextâ€generation quantum theory of atoms in molecules for the S₁/S₀ conical intersections in dynamics trajectories of a lightâ€driven rotary molecular motor. International Journal of Quantum Chemistry, 2020, 120, e26062.	2.0	12
23	Nextâ€generation QTAIM for scoring molecular wires in Eâ€fields for molecular electronic devices. Journal of Computational Chemistry, 2020, 41, 913-921.	3.3	12
24	Understanding the Polar Character Trend in a Series of Diels-Alder Reactions Using Molecular Quantum Similarity and Chemical Reactivity Descriptors. Journal of Quantum Chemistry, 2014, 2014, 1-19.	0.9	11
25	Quantum topology phase diagrams for the cisâ€and transâ€isomers of the cyclic contryphanâ€5m peptide. International Journal of Quantum Chemistry, 2014, 114, 1697-1706.	2.0	10
26	QTAIM and stress tensor interpretation of the (H₂ O)₅ potential energy surface. Journal of Computational Chemistry, 2016, 37, 2712-2721.	3.3	10
27	Molecular Quantum Similarity, Chemical Reactivity and Database Screening of 3D Pharmacophores of the Protein Kinases A, B and G from Mycobacterium tuberculosis. Molecules, 2017, 22, 1027.	3.8	10
28	Stress Tensor Eigenvector Following with Next-Generation Quantum Theory of Atoms in Molecules: Excited State Photochemical Reaction Path from Benzene to Benzvalene. Journal of Physical Chemistry A, 2019, 123, 8254-8264.	2.5	10
29	Chemical characterization and evaluation of the neuroprotective potential of Indigofera sessiliflora through in-silico studies and behavioral tests in scopolamine-induced memory compromised rats. Saudi Journal of Biological Sciences, 2021, 28, 4384-4398.	3.8	10
30	Beyond energetic and scalar measures: Next generation <scp>quantum theory of atoms in molecules</scp>. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	14.6	10
31	A 3â€D bonding perspective of the factors influencing the relative stability of the S1/S0conical intersections of the pentaâ€2,4â€dieniminium cation (PSB3). International Journal of Quantum Chemistry, 2019, 119, e25903.	2.0	9
32	Chiralityâ€“helicity of cumulenes: A nonâ€scalar charge density derived perspective. International Journal of Quantum Chemistry, 2022, 122, .	2.0	9
33	A QTAIM and stress tensor perspective of large-amplitude motions of the tetrasulfur tetranitride S₄N₄molecular graph. International Journal of Quantum Chemistry, 2016, 116, 1025-1039.	2.0	8
34	A conceptual DFT analysis of the plausible mechanism of some pericyclic reactions. Structural Chemistry, 2020, 31, 1745-1756.	2.0	8
35	Fatigue and fatigue resistance in S 1 excited state diarylethenes in electric fields. International Journal of Quantum Chemistry, 2021, 121, e26527.	2.0	8
36	Control of chirality, bond flexing and anharmonicity in an electric field. International Journal of Quantum Chemistry, 2021, 121, e26793.	2.0	8

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37	Chirality without Stereoisomers: Insight fromÂthe Helical Response of Bond Electrons. ChemPhysChem, 2021, 22, 1989-1995.	2.1	8
38	Mathematical Analysis of a Series of 4-Acetylamino-2-(3,5-dimethylpyrazol-1-yl)-6-pyridylpyrimidines: A Simple Way to Relate Quantum Similarity to Local Chemical Reactivity Using the Gaussian Orbitals Localized Theory. Journal of Theoretical Chemistry, 2014, 2014, 1-13.	1.5	7
39	The role of weak interactions in characterizing peptide folding preferences using a QTAIM interpretation of the Ramachandran plot (Ï•â€Ï‰). International Journal of Quantum Chemistry, 2018, 118, e25456.	2.0	7
40	An explanation of the unusual strength of the <scp>hydrogen bond</scp> in small water clusters. International Journal of Quantum Chemistry, 2020, 120, e26361.	2.0	7
41	Microwave-assisted synthesis, biological assessment, and molecular modeling of aza-heterocycles: Potential inhibitory capacity of cholinergic enzymes to Alzheimer's disease. Journal of Molecular Structure, 2021, 1224, 129307.	3.6	7
42	A vectorâ€based representation of the chemical bond for predicting competitive and noncompetitive torquoselectivity of thermal ringâ€opening reactions. International Journal of Quantum Chemistry, 2018, 118, e25707.	2.0	6
43	Flip rearrangement in the water pentamer: Analysis of electronic structure. International Journal of Quantum Chemistry, 2020, 120, e26124.	2.0	6
44	Analyzing torquoselectivity in a series of unusual ringâ€opening reactions through bond reactivity indices and the adaptive natural density partitioning method. International Journal of Quantum Chemistry, 2018, 118, e25778.	2.0	5
45	A vectorâ€based representation of the chemical bond for the normal modes of benzene. International Journal of Quantum Chemistry, 2018, 118, e25698.	2.0	5
46	Quantum mechanics and 3D-QSAR studies on thienopyridine analogues: inhibitors of IKKÎ². Heliyon, 2020, 6, e04125.	3.2	5
47	Discerning torquoselectivity in a series of cyclobutene <scp>ringâ€opening</scp> reactions using quantum theory of atoms in molecules and stress tensor. International Journal of Quantum Chemistry, 2022, 122, e26826.	2.0	5
48	Bond flexing, twisting, anharmonicity and responsivity for the infraredâ€active modes of benzene. International Journal of Quantum Chemistry, 2021, 121, e26584.	2.0	5
49	Hydroxyl-assisted selective epoxidation of perillyl alcohol with hydrogen peroxide by vanadium-substituted phosphotungstic acid hinged on imidazolyl activated carbon. New Journal of Chemistry, 2022, 46, 6636-6645.	2.8	5
50	Analyzing the substitution effect on the CoMFA results within the framework of density functional theory (DFT). Journal of Molecular Modeling, 2016, 22, 164.	1.8	4
51	New insights about electronic mechanism of electrocyclic reactions: theoretical study about stereoselectivity in cyclobutenes. Heliyon, 2021, 7, e06675.	3.2	4
52	New insights of QTAIM and stress tensor to finding non-competitive/competitive torquoselectivity of cyclobutene. Journal of Chemical Physics, 2021, 155, 204305.	3.0	4
53	Next generation quantum theory of atoms in molecules for the design of emitters exhibiting thermally activated delayed fluorescence with laser irradiation. Journal of Computational Chemistry, 2022, 43, 206-214.	3.3	4
54	Quantum topological resolution of catalyst proficiency. International Journal of Quantum Chemistry, 2015, 115, 875-883.	2.0	3

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55	Discerning the thermal cyclotrimerizations of fluoro- and chloroacetylenes through ELF, NBO descriptors and QTAIM analysis: pseudodiradical character. Heliyon, 2020, 6, e04441.	3.2	3
56	The chirality of isotopomers of glycine compared using nextâ€generation <scp>QTAIM</scp>. International Journal of Quantum Chemistry, 0, , .	2.0	3
57	Exploring the maximum Fukui function sites with the frontier-controlled soft-soft reactions using 1,3-dipolar cycloaddition reactions of nitrilium betaines. Journal of Molecular Modeling, 2022, 28, 116.	1.8	2
58	New molecular target insights about protein kinases of the Plasmodium falciparum. Using molecular docking and DFT-based reactivity descriptors. Journal of Theoretical and Computational Chemistry, 2017, 16, 1750076.	1.8	1
59	New insights about the serine/threonine protein kinase substrates from Mycobacterium tuberculosis using molecular docking, quantum similarity analysis and DFT calculations. F1000Research, 0, 10, 66.	1.6	0
60	Single crystal structure, thermal stability and theoretical studies of ethyl 4-(4-(dimethylamino)phenyl)-3,6-dimethyl-1-phenyl-1H-pyrazolo[3,4-b]pyridine-5-carboxylate. Journal of Molecular Structure, 2022, 1260, 132826.	3.6	0