Mar Ros-Gutirrez

List of Publications by Citations

84 papers	1,686 citations	19 h-index	38 g-index
90 ext. papers	2,116 ext. citations	3.2 avg, IF	5.81 L-index

#	Paper	IF	Citations
84	Applications of the Conceptual Density Functional Theory Indices to Organic Chemistry Reactivity. *Molecules*, **2016**, 21,	4.8	475
83	Unravelling the Mysteries of the [3+2] Cycloaddition Reactions. *European Journal of Organic Chemistry*, **2019**, 2019, 267-282	3.2	102
82	A Molecular Electron Density Theory Study of the Reactivity and Selectivities in [3 + 2] Cycloaddition Reactions of C,N-Dialkyl Nitrones with Ethylene Derivatives. *Journal of Organic Chemistry*, **2018**, 83, 2182-2197	4.2	72
81	A molecular electron density theory study of the participation of tetrazines in aza-Diels-Alder reactions.. *RSC Advances*, **2020**, 10, 15394-15405	3.7	57
80	How does the global electron density transfer diminish activation energies in polar cycloaddition reactions? A Molecular Electron Density Theory study. *Tetrahedron*, **2017**, 73, 1718-1724	2.4	52
79	A new model for C□□ bond formation processes derived from the Molecular Electron Density Theory in the study of the mechanism of [3+2] cycloaddition reactions of carbenoid nitrile ylides with electron-deficient ethylenes. *Tetrahedron*, **2016**, 72, 1524-1532	2.4	52
78	A Molecular Electron Density Theory Study of the Reactivity of Azomethine Imine in [3+2] Cycloaddition Reactions. *Molecules*, **2017**, 22,	4.8	48
77	The Mysticism of Pericyclic Reactions: A Contemporary Rationalisation of Organic Reactivity Based on Electron Density Analysis. *European Journal of Organic Chemistry*, **2018**, 2018, 1107-1120	3.2	47
76	A bonding evolution theory study of the mechanism of [3+2] cycloaddition reactions of nitrones with electron-deficient ethylenes. *RSC Advances*, **2015**, 5, 58464-58477	3.7	43
75	Non-classical CH?O hydrogen-bond determining the regio- and stereoselectivity in the [3 + 2] cycloaddition reaction of (Z)-C-phenyl-N-methylnitrone with dimethyl 2-benzylidenecyclopropane-1,1-dicarboxylate. A topological electron-density study. *RSC Advances*, **2015**, 5, 99299-99311	3.7	29
74	Unveiling the Reactivity of Cyclic Azomethine Ylides in [3+2] Cycloaddition Reactions within the Molecular Electron Density Theory. *European Journal of Organic Chemistry*, **2020**, 2020, 5938-5948	3.2	29
73	A molecular electron density theory study of the [3 + 2] cycloaddition reaction of nitrones with ketenes. *Organic and Biomolecular Chemistry*, **2017**, 15, 1618-1627	3.9	27
72	A Molecular Electron Density Theory Study of the Role of the Copper Metalation of Azomethine Ylides in [3 + 2] Cycloaddition Reactions. *Journal of Organic Chemistry*, **2018**, 83, 10959-10973	4.2	24
71	Unravelling the mechanism of the ketene-imine Staudinger reaction. An ELF quantum topological analysis. *RSC Advances*, **2015**, 5, 37119-37129	3.7	22
70	A Molecular Electron Density Theory Study of the Chemoselectivity, Regioselectivity, and Diastereofacial Selectivity in the Synthesis of an Anticancer Spiroisoxazoline derived from □Santonin. *Molecules*, **2019**, 24,	4.8	21
69	Understanding the reactivity and regioselectivity of [3 + 2] cycloaddition reactions between substituted nitrile oxides and methyl acrylate. A molecular electron density theory study. *International Journal of Quantum Chemistry*, **2017**, 117, e25451	2.1	21
68	A DFT study of the ionic [2+2] cycloaddition reactions of keteniminium cations with terminal acetylenes. *Tetrahedron*, **2015**, 71, 2421-2427	2.4	20

67	Unveiling the Lewis Acid Catalyzed Diels-Alder Reactions Through the Molecular Electron Density Theory. *Molecules*, **2020**, 25,	4.8	20
66	Understanding the carbenoid-type reactivity of nitrile ylides in [3+2] cycloaddition reactions towards electron-deficient ethylenes: a molecular electron density theory study. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	20
65	A molecular electron density theory study of the [3 + 2] cycloaddition reaction of nitrones with strained allenes. *RSC Advances*, **2017**, 7, 26879-26887	3.7	19
64	Unveiling the Different Chemical Reactivity of Diphenyl Nitrilimine and Phenyl Nitrile Oxide in [3+2] Cycloaddition Reactions with (R)-Carvone through the Molecular Electron Density Theory. *Molecules*, **2020**, 25,	4.8	19
63	A molecular electron density theory study of the enhanced reactivity of aza aromatic compounds participating in Diels-Alder reactions. *Organic and Biomolecular Chemistry*, **2020**, 18, 292-304	3.9	19
62	Steric interactions controlling the syn diastereofacial selectivity in the [3□+□2] cycloaddition reaction between acetonitrile oxide and 7-oxanorborn-5-en-2-ones: A molecular electron density theory study. *Journal of Physical Organic Chemistry*, **2017**, 30, e3710	2.1	18
61	The carbenoid-type reactivity of simplest nitrile imine from a molecular electron density theory perspective. *Tetrahedron*, **2019**, 75, 1961-1967	2.4	18
60	A molecular electron density theory study of the [3□+□2] cycloaddition reaction between an azomethine imine and electron deficient ethylenes. *Journal of Physical Organic Chemistry*, **2018**, 31, e3830	2.1	18
59	Understanding the domino reaction between 1-diazopropan-2-one and 1,1-dinitroethylene. A molecular electron density theory study of the [3 + 2] cycloaddition reactions of diazoalkanes with electron-deficient ethylenes. *RSC Advances*, **2017**, 7, 15586-15595	3.7	17
58	Understanding the high reactivity of carbonyl compounds towards nucleophilic carbenoid intermediates generated from carbene isocyanides. *RSC Advances*, **2015**, 5, 84797-84809	3.7	17
57	Understanding the [2n+2n] reaction mechanism between a carbenoid intermediate and CO2. *Molecular Physics*, **2016**, 114, 1374-1391	1.7	17
56	A DFT study of the mechanism and selectivities of the [3□+□2] cycloaddition reaction between 3-(benzylideneamino)oxindole and trans-□nitrostyrene. *Journal of Physical Organic Chemistry*, **2017**, 30, e3637	2.1	17
55	A DFT study of [3+2] cycloaddition reactions of an azomethine imine with N-vinyl pyrrole and N-vinyl tetrahydroindole. *Journal of Molecular Graphics and Modelling*, **2016**, 70, 296-304	2.8	16
54	A molecular electron density theory study of [3 + 2] cycloaddition reactions of chiral azomethine ylides with □nitrostyrene. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	16
53	A molecular electron density theory study of the Lewis acid□catalyzed decomposition reaction of nitroethyl benzoate using aluminum derivatives. *Journal of Physical Organic Chemistry*, **2019**, 32, e3938	2.1	15
52	Aromaticity in Pericyclic Transition State Structures? A Critical Rationalisation Based on the Topological Analysis of Electron Density. *ChemistrySelect*, **2016**, 1, 6026-6039	1.8	14
51	A DFT study of the mechanism of Br□sted acid catalysed Povarov reactions. *Tetrahedron*, **2015**, 71, 9339-9345	2.4	13
50	Understanding the stereoselectivity in Br□sted acid catalysed Povarov reactions generating cis/trans CF3-substituted tetrahydroquinolines: a DFT study. *RSC Advances*, **2016**, 6, 17064-17073	3.7	13

49	An MEDT study of the carbenoid-type [3 + 2] cycloaddition reactions of nitrile ylides with electron-deficient chiral oxazolidinones. *Organic and Biomolecular Chemistry*, **2016**, 14, 10427-10436	3.9	13
48	Understanding the molecular mechanism of the [3 + 2] cycloaddition reaction of benzonitrile oxide toward electron-rich N-vinylpyrrole: a DFT study. *Journal of Physical Organic Chemistry*, **2016**, 29, 368-376	2.1	11
47	Understanding the mechanism of the decomposition reaction of nitroethyl benzoate through the Molecular Electron Density Theory. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	10
46	Molecular Electron Density Theory Study of Fused Regioselectivity in the Intramolecular [3+2] Cycloaddition Reaction of Cyclic Nitrones. *ChemistrySelect*, **2018**, 3, 5412-5420	1.8	10
45	Understanding the reaction mechanism of the Lewis acid (MgBr2)-catalysed [3+2] cycloaddition reaction between C-methoxycarbonyl nitrone and 2-propen-1-ol: a DFT study. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	9
44	A molecular electron density theory study of the chemo- and regioselective [3 + 2] cycloaddition reactions between trifluoroacetonitrile N-oxide and thioketones. *Chemical Physics*, **2018**, 501, 128-137	2.3	9
43	A Molecular Electron Density Theory Study of the Competitiveness of Polar Diels?Alder and Polar Alder-ene Reactions. *Molecules*, **2018**, 23,	4.8	9
42	Unveiling the high reactivity of cyclohexynes in [3 + 2] cycloaddition reactions through the molecular electron density theory. *Organic and Biomolecular Chemistry*, **2019**, 17, 498-508	3.9	8
41	Are one-step aromatic nucleophilic substitutions of non-activated benzenes concerted processes?. *Organic and Biomolecular Chemistry*, **2019**, 17, 8185-8193	3.9	8
40	Understanding the Origin of the Regioselectivity in Non-Polar [3+2] Cycloaddition Reactions through the Molecular Electron Density Theory. *Organics*, **2020**, 1, 19-35	9	8
39	Experimental and Theoretical MEDT Study of the Thermal [3+2] Cycloaddition Reactions of Aryl Azides with Alkyne Derivatives. *ChemistrySelect*, **2018**, 3, 1215-1223	1.8	7
38	A combined experimental and theoretical study of the thermal [3+2] cycloaddition of carbonyl ylides with activated alkenes. *Journal of Molecular Structure*, **2018**, 1157, 276-287	3.4	7
37	Synthesis, molecular structure and stability of fused bicyclic 4-1,2,4-oxadiazoline Pt(II) complexes. *Polyhedron*, **2015**, 98, 55-63	2.7	7
36	On the nature of organic electron density transfer complexes within molecular electron density theory. *Organic and Biomolecular Chemistry*, **2019**, 17, 6478-6488	3.9	6
35	An MEDT study of the mechanism and selectivities of the [3+2] cycloaddition reaction of tomentosin with benzonitrile oxide. *International Journal of Quantum Chemistry*, **2019**, 119, e25980	2.1	6
34	A molecular electron density theory investigation of the molecular mechanism, regioselectivity, stereoselectivity and chemoselectivity of cycloaddition reaction between acetonitrile N-oxide and 2,5-dimethyl-2H-[1,2,3]diazarsole. *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	6
33	DFT exploration of [3 + 2] cycloaddition reaction of 1-phosphorinium-3-olate and 1-methylphosphorinium-3-olate with methyl methacrylate.. *RSC Advances*, **2018**, 8, 27406-27416	3.7	6
32	Electrophilic activation of CO2 in cycloaddition reactions towards a nucleophilic carbenoid intermediate: new defying insights from the Molecular Electron Density Theory. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	6

31	Unveiling the high reactivity of benzyne in the formal [3+2] cycloaddition reactions towards thioamides through the Molecular Electron Density Theory. *Tetrahedron*, **2020**, 76, 131458	2.4	6
30	A molecular electron density theory study of the mechanism, chemo- and stereoselectivity of the epoxidation reaction of -carvone with peracetic acid.. *RSC Advances*, **2019**, 9, 28500-28509	3.7	5
29	Deciphering the Mechanism of Silver Catalysis of "Click" Chemistry in Water by Combining Experimental and MEDT Studies. *Catalysts*, **2020**, 10, 956	4	5
28	Intrinsic relative nucleophilicity of indoles. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	5
27	A Molecular Electron Density Theory Study of the Synthesis of Spirobipyrazolines through the Domino Reaction of Nitrilimines with Allenoates. *Molecules*, **2019**, 24,	4.8	5
26	Understanding the Mechanism of Nitrobenzene Nitration with Nitronium Ion: A Molecular Electron Density Theory Study. *ChemistrySelect*, **2019**, 4, 13313-13319	1.8	5
25	Unveiling the Unexpected Reactivity of Electrophilic Diazoalkanes in [3+2] Cycloaddition Reactions within Molecular Electron Density Theory. *Chemistry*, **2021**, 3, 74-93	2.1	5
24	Understanding the Participation of Fluorinated Azomethine Ylides in Carbenoid-Type [3 + 2] Cycloaddition Reactions with Ynal Systems: A Molecular Electron Density Theory Study. *Journal of Organic Chemistry*, **2021**, 86, 12644-12653	4.2	5
23	Copper(I)-catalysed regioselective synthesis of pyrazolo[5,1-c]-1,2,4-triazoles: A DFT mechanistic study. *Tetrahedron*, **2017**, 73, 4653-4662	2.4	4
22	The Participation of 3,3,3-Trichloro-1-nitroprop-1-ene in the [3 + 2] Cycloaddition Reaction with Selected Nitrile -Oxides in the Light of the Experimental and MEDT Quantum Chemical Study. *Molecules*, **2021**, 26,	4.8	4
21	Understanding the Influence of the Trifluoromethyl Group on the Selectivities of the [3+2] Cycloadditions of Thiocarbonyl S-methanides with Unsaturated Ketones. A MEDT study. *ChemistrySelect*, **2020**, 5, 12791-12806	1.8	4
20	Aziridination of Aromatic Aldimines Through Stabilized Ammonium Ylides: A Molecular Electron Density Theory Study. *European Journal of Organic Chemistry*, **2019**, 2019, 1605-1613	3.2	4
19	A molecular electron density theory study of the insertion of CO into frustrated Lewis pair boron-amidines: a [4 + 1] cycloaddition reaction. *Dalton Transactions*, **2019**, 48, 9214-9224	4.3	3
18	Understanding the domino reactions of alkyne-tethered N-tosylhydrazones yielding fused polycyclic pyrazoles. An MEDT study. *Tetrahedron*, **2019**, 75, 2807-2816	2.4	3
17	Understanding the role of the trifluoromethyl group in reactivity and regioselectivity in [3+2] cycloaddition reactions of enol acetates with nitrones. A DFT study. *Journal of Molecular Modeling*, **2015**, 21, 104	2	3
16	An investigation of the molecular mechanism, chemoselectivity and regioselectivity of cycloaddition reaction between acetonitrile N-Oxide and 2,5-dimethyl-2H-[1,2,3]diazaphosphole: a MEDT study. *Journal of Chemical Sciences*, **2019**, 131, 1	1.8	3
15	A Molecular Electron Density Theory Study of the Lewis Acid Catalyzed [3+2] Cycloaddition Reactions of Nitrones with Nucleophilic Ethylenes. *European Journal of Organic Chemistry*, **2022**, 2022,	3.2	3
14	Mpro-SARS-CoV-2 Inhibitors and Various Chemical Reactivity of 1-Bromo- and 1-Chloro-4-vinylbenzene in [3 + 2] Cycloaddition Reactions. *Organics*, **2021**, 2, 1-16	9	3

13	Unveiling the Different Reactivity of Bent and Linear Three-Atom-Components Participating in [3 + 2] Cycloaddition Reactions. *Organics*, **2021**, 2, 274-286	9	3
12	Application of Reactivity Indices in the Study of Polar D iels□A lder Reactions **2022**, 481-502		3
11	[3+2] Cycloaddition reaction of 1H-phosphorinium-3-olate and 1-methylphosphorinium-3-olate with methyl acrylate: A DFT study. *Computational and Theoretical Chemistry*, **2016**, 1087, 36-47	2	2
10	Divulging the various chemical reactivity of trifluoromethyl-4-vinyl-benzene as well as methyl-4-vinyl-benzene in [3+2] cycloaddition reactions. *Journal of Molecular Graphics and Modelling*, **2021**, 102, 107760	2.8	2
9	Unveiling the regioselectivity in electrophilic aromatic substitution reactions of deactivated benzenes through molecular electron density theory. *New Journal of Chemistry*, **2021**, 45, 13626-13638	3.6	2
8	Understanding the Intramolecular Diels-Alder Reactions of N-Substituted N-Allyl-Furfurylamines: An MEDT Study. *ChemistrySelect*, **2017**, 2, 9736-9743	1.8	1
7	A DFT Study of the Conversion of Ptaquiloside, a Bracken Fern Carcinogen, to Pterosin B in Neutral and Acidic Aqueous Medium. *ChemistrySelect*, **2017**, 2, 8178-8186	1.8	1
6	Unveiling the Ionic Diels-Alder Reactions within the Molecular Electron Density Theory. *Molecules*, **2021**, 26,	4.8	1
5	Understanding the different reactivity of ()- and ()-□itrostyrenes in [3+2] cycloaddition reactions. An MEDT study.. *RSC Advances*, **2021**, 11, 9698-9708	3.7	1
4	A molecular electron density theory study of the [3 + 2] cycloaddition reaction of 1,4-diphosphorinium-3-olates with methyl acrylate and methyl methacrylate. *Theoretical Chemistry Accounts*, **2020**, 139, 1	1.9	0
3	Unveiling the Intramolecular Ionic Diels□Alder Reactions within Molecular Electron Density Theory. *Chemistry*, **2021**, 3, 834-853	2.1	
2	The catalytic effects of a thiazolium salt in the oxa-Diels-Alder reaction between benzaldehyde and Danishefsky's diene: a molecular electron density theory study. *Organic and Biomolecular Chemistry*, **2021**, 19, 9306-9317	3.9	
1	Selectivity: An Electron Density Perspective **2022**, 187-208		