

Jorge Ignacio MartÃ-nez-Araya

List of Publications by Year in descending order

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42
papers

1,270
citations

566801

15
h-index

360668

35
g-index

43
all docs

43
docs citations

43
times ranked

875
citing authors

#	ARTICLE	IF	CITATIONS
1	An electrostatic interaction correction for improved crystal density prediction. <i>Molecular Physics</i> , 2009, 107, 2095-2101.	0.8	365
2	Why is the dual descriptor a more accurate local reactivity descriptor than Fukui functions?. <i>Journal of Mathematical Chemistry</i> , 2015, 53, 451-465.	0.7	151
3	Local reactivity descriptors from degenerate frontier molecular orbitals. <i>Chemical Physics Letters</i> , 2009, 478, 310-322.	1.2	83
4	An electrostatic correction for improved crystal density predictions of energetic ionic compounds. <i>Molecular Physics</i> , 2010, 108, 1391-1396.	0.8	75
5	Energy and chemical force profiles from the Marcus equation. <i>Chemical Physics Letters</i> , 2004, 392, 132-139.	1.2	50
6	Explaining reaction mechanisms using the dual descriptor: a complementary tool to the molecular electrostatic potential. <i>Journal of Molecular Modeling</i> , 2013, 19, 2715-2722.	0.8	44
7	Revisiting caffeine's capabilities as a complexation agent to silver cation in mining processes by means of the dual descriptor: a conceptual DFT approach. <i>Journal of Molecular Modeling</i> , 2012, 18, 4299-4307.	0.8	41
8	The reaction force. A scalar property to characterize reaction mechanisms. <i>Journal of Mathematical Chemistry</i> , 2009, 45, 911-927.	0.7	39
9	Theoretical Study of Adsorption of Sarin and Soman on Tetrahedral Edge Clay Mineral Fragments. <i>Journal of Physical Chemistry B</i> , 2006, 110, 21175-21183.	1.2	37
10	Computational Nanochemistry Report on the Oxidation Conceptual DFT Indices and Chemical Reactivity. <i>Journal of Physical Chemistry B</i> , 2013, 117, 6339-6351.	1.2	35
11	On the Nature of the Active Site in bis(imino)Pyridyl Iron, a Catalyst for Olefin Polymerization. <i>Journal of Physical Chemistry C</i> , 2008, 112, 5023-5028.	1.5	34
12	Effect of the exchange-correlation functional on the synchronicity/nonsynchronicity in bond formation in Diels-Alder reactions: a reaction force constant analysis. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 7412-7428.	1.3	31
13	QSAR model for ethylene polymerisation catalysed by supported bis(imino)pyridine iron complexes. <i>Polymer</i> , 2007, 48, 7672-7678.	1.8	30
14	The dual descriptor to measure local reactivity on Buckminster fullerenes: an analysis within the framework of conceptual DFT. <i>Journal of Molecular Modeling</i> , 2010, 16, 1825-1832.	0.8	29
15	Towards the rationalization of catalytic activity values by means of local hyper-softness on the catalytic site: a criticism about the use of net electric charges. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 29764-29775.	1.3	17
16	Computational Nutraceuticals: Chemical Reactivity Properties of the Flavonoid Naringin by Means of Conceptual DFT. <i>Journal of Chemistry</i> , 2013, 2013, 1-8.	0.9	16
17	A generalized operational formula based on total electronic densities to obtain 3D pictures of the dual descriptor to reveal nucleophilic and electrophilic sites accurately on closed-shell molecules. <i>Journal of Computational Chemistry</i> , 2016, 37, 2279-2303.	1.5	16
18	A theoretical assessment of antioxidant capacity of flavonoids by means of local hyper-softness. <i>Arabian Journal of Chemistry</i> , 2018, 11, 554-563.	2.3	16

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19	The dual descriptor: Working equations applied on electronic open-shell molecular systems. <i>Chemical Physics Letters</i> , 2011, 506, 104-111.	1.2	15
20	The antioxidant capacity of myricetin. A molecular electrostatic potential analysis based on DFT calculations. <i>Chemical Physics Letters</i> , 2022, 801, 139708.	1.2	15
21	The Mechanism of Ethylene Polymerization Reaction Catalyzed by Group IVB Metallocenes. A Rational Analysis Through the Use of Reaction Force. <i>Journal of Physical Chemistry C</i> , 2012, 116, 21318-21325.	1.5	14
22	Explaining Some Anomalies in Catalytic Activity Values in Some Zirconocene Methyl Cations: Local Hyper-Softness. <i>Journal of Physical Chemistry C</i> , 2013, 117, 24773-24786.	1.5	12
23	Scrutinizing the substituent effect on Mo-based electrocatalysts for molecular hydrogen release through axial π -equatorial decomposition: a DFT study. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16601-16614.	1.3	12
24	Reaction Electronic Flux as a Fluctuation of Relative Interatomic Electronic Populations. <i>Journal of Physical Chemistry C</i> , 2015, 119, 3040-3049.	1.5	11
25	Assessment of a set of twelve density functionals to estimate the global reactivity of myricetin through the Koopmans π theorem. <i>Chemical Physics Letters</i> , 2019, 715, 354-359.	1.2	11
26	Theoretical insights into the linear relationship between α and ν values and vibrational frequencies. <i>Chemical Physics Letters</i> , 2022, 803, 139746.	1.2	10
27	1,3-Dipolar Cycloadditions by a Unified Perspective Based on Conceptual and Thermodynamics Models of Chemical Reactivity. <i>Journal of Physical Chemistry A</i> , 2021, 125, 801-815.	1.1	8
28	The substituent effect from the perspective of local hyper-softness. An example applied on normeloxicam, meloxicam and 4-meloxicam: Non-steroidal anti-inflammatory drugs. <i>Chemical Physics Letters</i> , 2015, 618, 162-167.	1.2	7
29	A statistical thermodynamics view of electron density polarisation: application to chemical selectivity. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 23553-23562.	1.3	7
30	A 3D visualization of the substituent effect. <i>Journal of Molecular Modeling</i> , 2018, 24, 31.	0.8	6
31	Solvent effect on the degree of (a)synchronicity in polar Diels-Alder reactions from the perspective of the reaction force constant analysis. <i>Journal of Molecular Modeling</i> , 2018, 24, 33.	0.8	6
32	Assessment of ten density functionals through the use of local hyper-softness to get insights about the catalytic activity. <i>Journal of Molecular Modeling</i> , 2018, 24, 42.	0.8	5
33	The importance of diffuse functions in basis sets to produce reliable 3D pictures of dual descriptor. <i>Chemical Physics Letters</i> , 2019, 724, 29-34.	1.2	5
34	Physicochemical and Theoretical Characterization of a New Small Non-Metal Schiff Base with a Differential Antimicrobial Effect against Gram-Positive Bacteria. <i>International Journal of Molecular Sciences</i> , 2022, 23, 2553.	1.8	5
35	Possible Use of Group 4 Metallocene Methyl Cations as Potential Neutralizers for FOX-7. <i>Propellants, Explosives, Pyrotechnics</i> , 2014, 39, 890-896.	1.0	3
36	The Dual Descriptor Reveals the Janus-Faced Behaviour of Diiodine. <i>Frontiers in Chemistry</i> , 2022, 10, 869110.	1.8	3

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37	An intermediate level of approximation for computing the dual descriptor. Journal of Molecular Modeling, 2013, 19, 2811-2820.	0.8	2
38	KID Procedure Applied on the $[(PY)_5Me_2]MoO^{+}$ Complex. ACS Omega, 2020, 5, 30549-30555.	1.6	2
39	Analysis in silico of chemical reactivity employing the local hypersoftness in some classic aromatic compounds, boron aromatic clusters and all-metal aromatic clusters. Journal of Computational Chemistry, 2022, 43, 29-42.	1.5	1
40	The density polarization reveals directions of electron displacements due to the substituent effect: Analysis performed on a metal-organic Mo=Oxo catalyst. Journal of Computational Chemistry, 2021, 42, 1118-1125.	1.5	0
41	Editorial: Endemic Plants: Experimental and Theoretical Insights Into Properties of Bioactive Metabolites With Therapeutic Potential. Frontiers in Chemistry, 2021, 9, 786865.	1.8	0
42	KID Procedure Applied on the $[(PYMe)MoO]$ Complex. ACS Omega, 2020, 5, 30549-30555.	1.6	0