Pablo Jaque

List of Publications by Year
in descending order

59 papers	2,212 citations	172386 29 h-index	223716 46 g-index
59 all docs	59 docs citations	59 times ranked	1863 citing authors

#	Article	IF	Citations
1	A deeper analysis of the role of synchronicity on the Bellâ€“Evansâ€“Polanyi plot in multibond chemical reactions: a path-dependent reaction force constant. Physical Chemistry Chemical Physics, 2022, 24, 14772-14779.	1.3	5
2	Automating the IRCâ€Analysis within Eyringpy. International Journal of Quantum Chemistry, 2021, 121, e26684.	1.0	7
3	1,3-Dipolar Cycloadditions by a Unified Perspective Based on Conceptual and Thermodynamics Models of Chemical Reactivity. Journal of Physical Chemistry A, 2021, 125, 801-815.	1.1	8
4	5-HT₂ Receptor Subfamily and the Halogen Bond Promise. Journal of Chemical Information and Modeling, 2021, 61, 5001-5012.	2.5	3
5	Real-Space Approach to the Reaction Force: Understanding the Origin of Synchronicity/Nonsynchronicity in Multibond Chemical Reactions. Journal of Physical Chemistry A, 2020, 124, 1959-1972.	1.1	12
6	DFT benchmark study of the Oâ€“O bond dissociation energy in peroxides validated with high-level ab initio calculations. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	6
7	Elucidating sensing mechanisms of a pyrene excimer-based calix[4]arene for ratiometric detection of Hg(<scp>ii</scp>) and Ag(<scp>i</scp>) and chemosensor behaviour as INHIBITION or IMPLICATION logic gates. RSC Advances, 2020, 10, 21963-21973.	1.7	14
8	Unusual Oxidative Dealkylation Strategy toward Functionalized Phenalenones as Singlet Oxygen Photosensitizers and Photophysical Studies. Journal of Organic Chemistry, 2020, 85, 10603-10616.	1.7	11
9	Reaction mechanism of hydrogen activation by frustrated Lewis pairs. Green Energy and Environment, 2019, 4, 20-28.	4.7	38
10	Scrutinizing the substituent effect on Mo-based electrocatalysts for molecular hydrogen release through axialâ€“equatorial decomposition: a DFT study. Physical Chemistry Chemical Physics, 2019, 21, 16601-16614.	1.3	12
11	Further understanding of the Ru-centered [2+2] cycloreversion/cycloaddition involved into the interconversion of ruthenacyclobutane using the Grubbs catalysts from a reaction force analysis. Journal of Molecular Modeling, 2019, 25, 305.	0.8	4
12	Unexpected intramolecular N-arylcyano-Î²-diketiminate cyclization in new aminoquinoline derivative complexes of aluminium for CO₂ fixation into cyclic carbonates. New Journal of Chemistry, 2019, 43, 12059-12068.	1.4	3
13	Effect of the exchangeâ€“correlation functional on the synchronicity/nonsynchronicity in bond formation in Dielsâ€“Alder reactions: a reaction force constant analysis. Physical Chemistry Chemical Physics, 2019, 21, 7412-7428.	1.3	31
14	Solvent effect on the degree of (a)synchronicity in polar Diels-Alder reactions from the perspective of the reaction force constant analysis. Journal of Molecular Modeling, 2018, 24, 33.	0.8	6
15	A systematic electronic structure study of the Oâ€“O bond dissociation energy of hydrogen peroxide and the electron affinity of the hydroxyl radical. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	7
16	Hydrogenation of Multiple Bonds by Geminal Aminoboraneâ€Based Frustrated Lewis Pairs. Chemistry - A European Journal, 2018, 24, 8833-8840.	1.7	32
17	Effect of Lewis acid bulkiness on the stereoselectivity of Dielsâ€“Alder reactions between acyclic dienes and Î±,Î²-enals. Organic Chemistry Frontiers, 2017, 4, 1390-1399.	2.3	29
18	New imidoyl-indazole platinum (II) complexes as potential anticancer agents: Synthesis, evaluation of cytotoxicity, cell death and experimental-theoretical DNA interaction studies. Journal of Inorganic Biochemistry, 2017, 174, 90-101.	1.5	8

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19	Deeper Insight into the Factors Controlling H₂ Activation by Geminal Aminoboraneâ€Based Frustrated Lewis Pairs. Chemistry - A European Journal, 2016, 22, 18801-18809.	1.7	52
20	Theoretical characterization of first and second generation Grubbs catalysts in styrene cross-metathesis reactions: insights from conceptual DFT. Catalysis Science and Technology, 2016, 6, 755-766.	2.1	16
21	Theoretical study of dibenzyl disulfide adsorption on Cu7 cluster as a first approximation to sulfur-induced copper corrosion process. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	9
22	Clean Singlet Oxygen Production by a Re^I Complex Embedded in a Flexible Self-Standing Polymeric Silsesquioxane Film. Journal of Physical Chemistry C, 2015, 119, 10148-10159.	1.5	32
23	A computational and conceptual DFT study on the mechanism of hydrogen activation by novel frustrated Lewis pairs. Physical Chemistry Chemical Physics, 2015, 17, 10715-10725.	1.3	20
24	Initiation stage of alkene metathesis: Insights from natural bond orbital and charge decomposition analyses. Chemical Physics Letters, 2015, 618, 174-181.	1.2	6
25	Insights into some Dielsâ€“Alder cycloadditions via the electrostatic potential and the reaction force constant. Computational and Theoretical Chemistry, 2015, 1053, 270-280.	1.1	21
26	Stability analysis of lithio-silicon Si10Li8 clusters: Planar bicyclic ring vs. three-dimensional structures. Chemical Physics Letters, 2014, 604, 72-76.	1.2	4
27	DFT Study on the Relative Stabilities of Substituted Ruthenacyclobutane Intermediates Involved in Olefin Cross-Metathesis Reactions and Their Interconversion Pathways. Organometallics, 2014, 33, 6065-6075.	1.1	31
28	Polarizability of neutral copper clusters. Journal of Molecular Modeling, 2014, 20, 2410.	0.8	13
29	Driving and retarding forces in a chemical reaction. Journal of Molecular Modeling, 2014, 20, 2351.	0.8	25
30	Complementarity of reaction force and electron localization function analyses of asynchronicity in bond formation in Dielsâ€“Alder reactions. Physical Chemistry Chemical Physics, 2014, 16, 6726.	1.3	62
31	Traditional and Ion-Pair Halogen-Bonded Complexes Between Chlorine and Bromine Derivatives and a Nitrogen-Heterocyclic Carbene. Journal of Physical Chemistry A, 2014, 118, 9552-9560.	1.1	38
32	Photoemission Spectra and Density Functional Theory Calculations of 3d Transition Metalâ€“Aqua Complexes (Tiâ€“Cu) in Aqueous Solution. Journal of Physical Chemistry B, 2014, 118, 6850-6863.	1.2	28
33	Perspectives on the reaction force constant. Journal of Molecular Modeling, 2013, 19, 4111-4118.	0.8	45
34	The reaction force constant as an indicator of synchronicity/nonsynchronicity in [4+2] cycloaddition processes. Physical Chemistry Chemical Physics, 2013, 15, 7311.	1.3	53
35	Fine structure in the transition region: reaction force analyses of water-assisted proton transfers. Journal of Molecular Modeling, 2013, 19, 2689-2697.	0.8	36
36	The reaction force constant: an indicator of the synchronicity in double proton transfer reactions. Physical Chemistry Chemical Physics, 2012, 14, 11125.	1.3	54

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37	Electronic activity in chelotropic and cycloaddition reactions. International Journal of Quantum Chemistry, 2012, 112, 2142-2153.	1.0	5
38	Theoretical analysis based on Xâ€“H bonding strength and electronic properties in red- and blue-shifting hydrogen-bonded Xâ€“Hâ‹¯Ï€ complexes. Physical Chemistry Chemical Physics, 2011, 13, 1552-1559.	1.3	33
39	Regioselectivity of Radical Additions to Substituted Alkenes: Insight from Conceptual Density Functional Theory. Journal of Organic Chemistry, 2010, 75, 4964-4974.	1.7	19
40	Regaining the Woodwardâ€“Hoffmann rules for chelotropic reactions via conceptual DFT. Canadian Journal of Chemistry, 2010, 88, 858-865.	0.6	16
41	A New View on the Spectrochemical and Nephelauxetic Series on the Basis of Spinâ€Polarized Conceptual DFT. ChemPhysChem, 2009, 10, 847-854.	1.0	15
42	Nucleophilicity and electrophilicity of silylenes from a molecular electrostatic potential and dual descriptor perspectives. Chemical Physics Letters, 2009, 470, 180-186.	1.2	17
43	Theoretical Study of the Regioselectivity of [2 + 2] Photocycloaddition Reactions of Acrolein with Olefins. Journal of Physical Chemistry A, 2009, 113, 332-344.	1.1	48
44	Analyzing Kullbackâ€“Leibler information profiles: an indication of their chemical relevance. Physical Chemistry Chemical Physics, 2009, 11, 476-482.	1.3	31
45	Reaction force constant and projected force constants of vibrational modes along the path of an intramolecular proton transfer reaction. Chemical Physics Letters, 2008, 456, 135-140.	1.2	80
46	The Study of Redox Reactions on the Basis of Conceptual DFT Principles: EEM and Vertical Quantities. Journal of Physical Chemistry A, 2008, 112, 6023-6031.	1.1	53
47	Computational Electrochemistry: The Aqueous Ru3+ | Ru2+Reduction Potential. Journal of Physical Chemistry C, 2007, 111, 5783-5799.	1.5	126
48	Can Electrophilicity Act as a Measure of the Redox Potential of Firstâ€Row Transition Metal Ions?. Chemistry - A European Journal, 2007, 13, 9331-9343.	1.7	55
49	Molecular Structure and Bonding of Copper Cluster Monocarbonyls CunCO (n= 1â^'9). Journal of Physical Chemistry B, 2006, 110, 6526-6536.	1.2	97
50	Reaction Force Analysis of the Effect of Mg(II) on the 1,3 Intramolecular Hydrogen Transfer in Thymine. Journal of Physical Chemistry A, 2006, 110, 9478-9485.	1.1	91
51	Connection between the average local ionization energy and the Fukui function. Chemical Physics Letters, 2005, 407, 143-146.	1.2	34
52	The reaction force: Three key points along an intrinsic reaction coordinate. Journal of Chemical Sciences, 2005, 117, 467-472.	0.7	122
53	The Formation of Neutral Copper Clusters from Experimental Binding Energies and Reactivity Descriptors. Journal of Physical Chemistry B, 2004, 108, 2568-2574.	1.2	30
54	Towards understanding the molecular internal rotations and vibrations and chemical reactions through the profiles of reactivity and selectivity indices: an ab initio SCF and DFT study. Molecular Physics, 2003, 101, 2841-2853.	0.8	42

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55	Characterization of copper clusters through the use of density functional theory reactivity descriptors. Journal of Chemical Physics, 2002, 117, 3208-3218.	1.2	186
56	Using Sanderson's Principle to Estimate Global Electronic Properties and Bond Energies of Hydrogen-Bonded Complexes. Journal of Physical Chemistry A, 2000, 104, 8955-8964.	1.1	57
57	Theoretical Study of the Double Proton Transfer in the CHXâ^'XHÂ·Â·Â·CHXâ^'XH (X = O, S) Complexes. Journal of Physical Chemistry A, 2000, 104, 995-1003.	1.1	114
58	Simultaneous determination of chlordiazepoxide and clidinium bromide in pharmaceutical formulations by derivative spectrophotometry. International Journal of Pharmaceutics, 1999, 189, 67-74.	2.6	33
59	Validity of the Minimum Polarizability Principle in Molecular Vibrations and Internal Rotations:Â An ab Initio SCF Study. Journal of Physical Chemistry A, 1999, 103, 9307-9312.	1.1	127