Soledad GutiÃ©rrez-Oliva

List of Publications by Year
in descending order

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49 papers	1,420 citations	331259 21 h-index	329751 37 g-index
51 all docs	51 docs citations	51 times ranked	835 citing authors

#	Article	IF	Citations
1	The reaction force: Three key points along an intrinsic reaction coordinate. Journal of Chemical Sciences, 2005, 117, 467-472.	0.7	122
2	The reaction force and the transition region of a reaction. Journal of Molecular Modeling, 2009, 15, 707-710.	0.8	101
3	Rationalization of Dielsâ€“Alder reactions through the use of the dual reactivity descriptor Î”f(r). Physical Chemistry Chemical Physics, 2008, 10, 7239.	1.3	94
4	On the Mechanism of Hydrogen Transfer in the HSCH(O) â‡Œ (S)CHOH and HSNO â‡Œ SNOH Reactions. Journal of Physical Chemistry A, 2005, 109, 1748-1751.	1.1	93
5	Analysis of two intramolecular proton transfer processes in terms of the reaction force. Journal of Chemical Physics, 2004, 121, 4570-4576.	1.2	78
6	Reaction Force Decomposition of Activation Barriers To Elucidate Solvent Effects. Journal of Physical Chemistry A, 2007, 111, 2455-2457.	1.1	71
7	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
8	The reaction electronic flux in chemical reactions. Science China Chemistry, 2011, 54, 1982-1988.	4.2	52
9	Energy, chemical potential and hardness profiles for the rotational isomerization of HOOH, HSOH and HSSH. Molecular Physics, 1999, 96, 61-70.	0.8	47
10	The reaction electronic flux: A new descriptor of the electronic activity taking place during a chemical reaction. Application to the characterization of the mechanism of the Schiffâ€™s base formation in the Maillard reaction. Computational and Theoretical Chemistry, 2010, 943, 121-126.	1.5	46
11	Relations between Potential Energy, Electronic Chemical Potential, and Hardness Profiles. Journal of Physical Chemistry A, 1997, 101, 4621-4627.	1.1	45
12	Theoretical Study on a Multicenter Model Based on Different Metal Oxidation States for the Bis(imino)pyridine Iron Catalysts in Ethylene Polymerization. Organometallics, 2009, 28, 5889-5895.	1.1	43
13	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
14	Perspectives on the Reaction Force. Advances in Quantum Chemistry, 2012, 64, 189-209.	0.4	36
15	On the Nature of the Active Site in bis(imino)Pyridyl Iron, a Catalyst for Olefin Polymerization. Journal of Physical Chemistry C, 2008, 112, 5023-5028.	1.5	34
16	Reaction Force Analysis of Solvent Effects in the Addition of HCl to Propene. Journal of Physical Chemistry A, 2009, 113, 6500-6503.	1.1	32
17	The mechanism of chemisorption of hydrogen atom on graphene: Insights from the reaction force and reaction electronic flux. Journal of Chemical Physics, 2014, 141, 134701.	1.2	27
18	Catalytic Mechanism of H2Activation by a Carbenoid Aluminum Complex. Journal of Physical Chemistry C, 2015, 119, 26598-26604.	1.5	27

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19	The mechanism of double proton transfer in dimers of uracil and 2â€thiouracilâ€"The reaction force perspective. Journal of Computational Chemistry, 2009, 30, 389-398.	1.5	26
20	A detailed analysis of the mechanism of a carbocationic triple shift rearrangement. Physical Chemistry Chemical Physics, 2015, 17, 9771-9779.	1.3	24
21	Double Gold Activation of 1â€Ethynylâ€2â€(Phenylethynyl)Benzene Toward 5â€‹exo‹/i›â€dig and 6â€‹endo‹/i›â€dig Cyclization Reactions. Chemistry - A European Journal, 2017, 23, 13360-13368.	1.7	21
22	Insights into the chemical meanings of the reaction electronic flux. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	20
23	ETSâ€NOCV Decomposition of the Reaction Force: The HCN/CNH Isomerization Reaction Assisted by Water. Journal of Computational Chemistry, 2017, 38, 2076-2087.	1.5	19
24	The torsional problem of oxalyl chloride: a challenge for theoretical methods. Chemical Physics Letters, 2004, 383, 435-440.	1.2	17
25	Revisiting the seemingly straightforward hydrogen cyanide/hydrogen isocyanide isomerisation. Molecular Physics, 2014, 112, 349-354.	0.8	17
26	Role of water in intramolecular proton transfer reactions of formamide and thioformamide. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	17
27	Insights into the Mechanism of Ground and Excited State Double Proton Transfer Reaction in Formic Acid Dimer. Journal of Physical Chemistry A, 2017, 121, 9531-9543.	1.1	16
28	The performance of methallyl nickel complexes and boron adducts in the catalytic activation of ethylene: a conceptual DFT perspective. Journal of Molecular Modeling, 2015, 21, 227.	0.8	14
29	Bridging the Gap between the Topological and Orbital Description of Hydrogen Bonding:Â The Case of the Formic Acid Dimer and Its Sulfur Derivatives. Journal of Physical Chemistry A, 2006, 110, 5102-5107.	1.1	13
30	The Role of Coâ€Activation and Ligand Functionalization in Neutral Methallyl Nickel(II) Catalysts for Ethylene Oligomerization and Polymerization. Chemistry - A European Journal, 2017, 23, 10167-10176.	1.7	13
31	Molecular hydrogen formation in the interstellar medium: the role of polycyclic aromatic hydrocarbons analysed by the reaction force and activation strain model. Monthly Notices of the Royal Astronomical Society, 2018, 481, 3052-3062.	1.6	13
32	Reversibility from DFT-Based Reactivity Indices: Intramolecular Side Reactions in the Polymerization of Poly(vinyl chloride). Journal of Physical Chemistry A, 2009, 113, 7899-7908.	1.1	11
33	Study of antiradical mechanisms with dihydroxybenzenes using reaction force and reaction electronic flux. Physical Chemistry Chemical Physics, 2017, 19, 14512-14519.	1.3	11
34	Reaction Electronic Flux Perspective on the Mechanism of the Zimmerman Di-Ï€-methane Rearrangement. Journal of Organic Chemistry, 2018, 83, 5969-5974.	1.7	11
35	An extension of the Marcus equation: the Marcus potential energy function. Journal of Molecular Modeling, 2018, 24, 104.	0.8	10
36	A Relation between Different Scales of Electrophilicity: Are the Scales Consistent Along a Chemical Reaction?. Journal of Physical Chemistry A, 2012, 116, 7074-7081.	1.1	9

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37	Why Low Valent Lead(II) Hydride Complex Would be a Better Catalyst for CO₂ Activation than Its 14 Group Analogues?. Journal of Physical Chemistry C, 2017, 121, 12127-12135.	1.5	9
38	Hydrogenation and hydration of carbon dioxide: a detailed characterization of the reaction mechanisms based on the reaction force and reaction electronic flux analyses. Journal of Molecular Modeling, 2019, 25, 16.	0.8	9
39	Chapter 7 Using the reactivity-selectivity descriptor Î” f(r) in organic chemistry. Theoretical and Computational Chemistry, 2007, , 101-117.	0.2	8
40	Symmetry-adapted reaction electronic flux in cycloaddition reactions. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	8
41	The effect of heteroatoms in carbonaceous surfaces: computational analysis of H chemisorption on to a PANH and Si-doped PAH. Monthly Notices of the Royal Astronomical Society, 2019, 490, 172-180.	1.6	7
42	Interacting Quantum Atoms Analysis of the Reaction Force: A Tool to Analyze Driving and Retarding Forces in Chemical Reactions. ChemPhysChem, 2021, 22, 1976-1988.	1.0	7
43	Insights into the Maillard reaction. The mechanism of Schiff's base formation from the reaction force perspective. Molecular Physics, 2009, 107, 1587-1596.	0.8	6
44	Theoretical study of the hydrogen abstraction from vitamin-E analogues. The usefulness of DFT descriptors. Journal of Molecular Modeling, 2011, 17, 593-598.	0.8	6
45	Enhanced reactivity of Lys182 explains the limited efficacy of biogenic amines in preventing the inactivation of glucose-6-phosphate dehydrogenase by methylglyoxal. Bioorganic and Medicinal Chemistry, 2011, 19, 1613-1622.	1.4	6
46	Effects of the ionization in the tautomerism of uracil: A reaction electronic flux perspective. Journal of Computational Chemistry, 2015, 36, 2135-2145.	1.5	6
47	Spectral Decomposition of the Reaction Force Constant. Journal of Physical Chemistry A, 2020, 124, 2372-2379.	1.1	6
48	Electropolymerization of 3â€²,4â€²-disubstituted 2,2â€²:5â€²,2â€³-terthiophene derivatives. A theoretical and photovoltaic characterization. Journal of Molecular Modeling, 2011, 17, 81-88.	0.8	4
49	The influence of the metal cations and microhydration on the reaction trajectory of the N3 â†” O2 thymine proton transfer: Quantum mechanical study. Journal of Computational Chemistry, 2017, 38, 2680-2692.	1.5	4