Angeles PeÃ±a-Gallego

List of Publications by Year
in descending order

57 papers	817 citations	516710 16 h-index	580821 25 g-index
59 all docs	59 docs citations	59 times ranked	875 citing authors

#	Article	IF	Citations
1	DFT conformational study of cysteine in gas phase and aqueous solution. Computational and Theoretical Chemistry, 2000, 498, 191-200.	1.5	64
2	Computational Study on the Characteristics of the Interaction in NaphthaleneÂ·Â·Â·(H₂X)_{n=1,2} (X = O, S) Clusters. Journal of Physical Chemistry A, 2008, 112, 6344-6350.	2.5	54
3	Intermolecular interactions and cooperative effects in acetonitrile clusters. An ab initio molecular orbital study. Computational and Theoretical Chemistry, 2000, 498, 21-28.	1.5	45
4	A DFT Study of the Boultonâ^'Katritzky Rearrangement of (5R)-4-Nitrosobenz[c]isoxazole and Its Anion:â€‰ Pseudopericyclic Reactions with Aromatic Transition States. Journal of Organic Chemistry, 2004, 69, 7013-7017.	3.2	41
5	DFT Study of Pericyclic and Pseudopericyclic Thermal Cheletropic Decarbonylations. Evaluation of Magnetic Properties. Journal of Organic Chemistry, 2003, 68, 8823-8830.	3.2	39
6	The Role of Aromaticity in the Planarity of Lumiflavin. Journal of Organic Chemistry, 2002, 67, 6347-6352.	3.2	34
7	Are Electrocyclization Reactions of (3Z)-1,3,5-Hexatrienone and Nitrogen Derivatives Pseudopericyclic? A DFT Study. Journal of Organic Chemistry, 2005, 70, 3921-3928.	3.2	34
8	Cation-Ï€ and anion-Ï€ interactions: Changes in aromaticity upon complexation. Chemical Physics Letters, 2008, 452, 49-53.	2.6	25
9	A Density Functional Theory Study on the Electrocyclization of 1,2,4,6-Heptatetraene Analogues: Converting a Pericyclic to a Pseudopericyclic Reaction. Chemistry - A European Journal, 2005, 11, 5966-5974.	3.3	24
10	Metallaaromatic biaryl atropisomers. Chemical Communications, 2018, 54, 10974-10976.	4.1	21
11	NMR spectroscopy for assessing cocaine-functional monomer interactions when preparing molecularly imprinted polymers. Microchemical Journal, 2019, 147, 813-817.	4.5	21
12	Characteristics of the interaction of azulene with water and hydrogen sulfide: A computational study. Journal of Chemical Physics, 2008, 129, 084305.	3.0	20
13	Nonstatistical effects in the unimolecular dissociation of the acetyl radical. Journal of Chemical Physics, 1999, 110, 11323-11334.	3.0	17
14	Dissociation of ethylene and several deuterated derivatives at 193 and 157 nm by direct classical trajectories. Chemical Physics Letters, 2002, 353, 418-425.	2.6	17
15	A DFT Study of the Concerted Cyclisation of 3-Azidopropenal to Isoxazole:Is it a Pseudopericyclic Reaction According to Its Magnetic Properties?. European Journal of Organic Chemistry, 2005, 2005, 3228-3232.	2.4	17
16	A DFT Study of the Pericyclic/Pseudopericyclic Character of Cycloaddition Reactions of Ethylene and Formaldehyde to Buta-1,3-dien-1-one and Derivatives. Journal of Physical Chemistry A, 2005, 109, 5636-5644.	2.5	17
17	Study of the ferroceneâ€“lithium cation interaction by DFT calculations: an in-depth analysis of the existence of a planetary system. Tetrahedron, 2009, 65, 2368-2371.	1.9	17
18	Effect of microhydration on the guanidiniumâ‹¯benzene interaction. Journal of Chemical Physics, 2011, 135, 214301.	3.0	17

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19	Spirobifluorene Metallaaromatics. Chemistry - A European Journal, 2019, 25, 13496-13499.	3.3	17
20	Distinct Helical Molecular Orbitals through Conformational Lock**. Chemistry - A European Journal, 2020, 26, 17342-17349.	3.3	17
21	A MP2 and DFT study of the aromatic character of polyphosphaphospholes. Is the pyramidality the only factor to take into consideration?. Journal of Molecular Modeling, 2011, 17, 1267-1272.	1.8	14
22	A DFT study of the [4+2] cycloadditions of conjugated ketenes (vinylketene, imidoylketene and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 6 properties. Tetrahedron, 2007, 63, 4937-4943.	1.9	13
23	Assessing the Reversed Exponential Decay of the Electrical Conductance in Molecular Wires: The Undeniable Effect of Static Electron Correlation. Nano Letters, 2019, 19, 7394-7399.	9.1	13
24	A Comparative Theoretical Study of the Pericyclic-pseudopericyclic Character in a Group of Cyclizations of Dienylketenes to Cyclohexadienones. Journal of Physical Chemistry A, 2007, 111, 2935-2940.	2.5	12
25	Kinetic study of the formation of <scp>N</scp>â€chloro compounds using <scp>N</scp>â€chlorosuccinimide. Journal of Physical Organic Chemistry, 2014, 27, 407-418.	1.9	12
26	Direct dynamics simulation of the methanethiol cation decomposition. Chemical Physics Letters, 2000, 324, 88-94.	2.6	11
27	Study of the interaction in clusters formed by phenol and CH3X (X=CN,F,Cl) molecules. Journal of Chemical Physics, 2008, 128, 194311.	3.0	11
28	A computational study of the mechanism of the unimolecular elimination of Î±,Î²-unsaturated aldehydes in the gas phase. Journal of Molecular Modeling, 2011, 17, 21-26.	1.8	11
29	An ab initio study of a model compound of penicillins. Computational and Theoretical Chemistry, 1999, 491, 177-185.	1.5	10
30	Theoretical study of the walk rearrangement in perfluorotetramethyl (Dewar thiophene) exo-S-oxide. Tetrahedron, 2007, 63, 2191-2198.	1.9	10
31	Computational study of the interaction of indole-like molecules with water and hydrogen sulfide. Journal of Chemical Physics, 2011, 135, 134310.	3.0	10
32	A quantum chemical study of aniline/ammonia clusters. Thermodynamic properties and frequency analysis. Computational and Theoretical Chemistry, 2000, 497, 105-113.	1.5	9
33	MRCI Calculation, Scaling of the External Correlation, and Modeling of Potential Energy Curves for HCl and OCl. Journal of Physical Chemistry A, 2000, 104, 6241-6246.	2.5	9
34	Clar Goblet and Aromaticity Driven Multiradical Nanographenes. Chemistry - A European Journal, 2020, 26, 16138-16143.	3.3	9
35	Dynamics of the cisâ€“trans isomerization and Clâ€“O dissociation of chlorine nitrite. Classical trajectory and statistical calculations. Physical Chemistry Chemical Physics, 2000, 2, 5393-5399.	2.8	8
36	Study of the interaction between aniline and CH3CN, CH3Cl and CH3F. Theoretical Chemistry Accounts, 2011, 128, 531-539.	1.4	8

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37	Key factors in the synthesis of polycyclic iridaaromatics via the methoxyalkenylcarbene pathway. Dalton Transactions, 2021, 50, 11216-11220.	3.3	8
38	Classical Trajectory Study of the Cisâ^'Trans Isomerization and Fâ^'O Dissociation of FONO. Journal of Physical Chemistry A, 1998, 102, 8708-8715.	2.5	7
39	The effect of spin polarization on the electron transport of molecular wires with diradical character. Physical Chemistry Chemical Physics, 2021, 23, 4777-4783.	2.8	7
40	A computational study of the electrocyclization of o-divinylbenzene and derivatives. Computational and Theoretical Chemistry, 2007, 811, 141-151.	1.5	6
41	Molecular recognition-based catalysis in nucleophilic aromatic substitution: a mechanistic study. New Journal of Chemistry, 2012, 36, 1519.	2.8	6
42	Detecting Molecular Plasmons by Means of Electron Density Descriptors. Journal of Physical Chemistry C, 2020, 124, 1585-1593.	3.1	6
43	Design and synthesis of chiral spirobifluorenes. Chirality, 2020, 32, 464-473.	2.6	6
44	A Tetracyanobutadiene Spirobifluorene: Synthesis, Enantiomeric Resolution and Chiroptical Properties. European Journal of Organic Chemistry, 2022, 2022, .	2.4	6
45	The unimolecular dissociation of the propionyl radical: A classical dynamics study. Journal of Chemical Physics, 2001, 114, 3546-3553.	3.0	5
46	Chiroptical Symmetry Analysis: Exciton Chirality-Based Formulae to Understand the Chiroptical Responses of Cn and Dn Symmetric Systems. Molecules, 2019, 24, 141.	3.8	5
47	Chemoselectivity on the synthesis of iridacycles: A theoretical and experimental study. Inorganica Chimica Acta, 2021, 517, 120189.	2.4	5
48	Product energy distributions from ethylene photodissociation at 193 nm: a DFT direct classical trajectory study. Chemical Physics Letters, 2003, 369, 1-7.	2.6	4
49	A theoretical study of the influence of BF3 on the reaction path of the [4+2] cycloaddition of vinylketene with formaldimine. Tetrahedron, 2007, 63, 11617-11621.	1.9	4
50	Comment on â€œA Theoretical Investigation of the Interactions between Water Molecules and Ionic Liquidsâ€• Journal of Physical Chemistry B, 2008, 112, 13465-13466.	2.6	3
51	Chiroptical Symmetry Analysis of Trianglimines: A Case Study. Symmetry, 2019, 11, 1245.	2.2	3
52	ON/OFF Spiroconjugation through Peripheral Functionalization: Impact on the Reactivity and Chiroptical Properties of Spirobifluorenes. ChemPlusChem, 2022, 87, e202100554.	2.8	3
53	A DFT study of a model compound of vitamin D. Computational and Theoretical Chemistry, 1999, 492, 143-150.	1.5	2
54	A MP2 and DFT study of the influence of complexation on the aromatic character of phosphole. Journal of Molecular Modeling, 2012, 18, 765-770.	1.8	2

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55	Unimolecular Electrical Rectification Understood Through Electron Deformation Orbitals. Journal of Physical Chemistry C, 2020, 124, 17924-17931.	3.1	1
56	Theoretical study of the decomposition of ethyl and ethyl 3-phenyl glycidate. Journal of Molecular Modeling, 2013, 19, 315-320.	1.8	0
57	Tracking the Transition from Pericyclic to Pseudopericyclic Reaction Mechanisms Using Multicenter Electron Delocalization Analysis: The [1,3] Sigmatropic Rearrangement. Journal of Physical Chemistry A, 2021, 125, 8337-8344.	2.5	0